Covariant Hamiltonian boundary conditions in General Relativity for spatially bounded spacetime regions.

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Abstract

We investigate the covariant Hamiltonian symplectic structure of General Relativity for spatially bounded regions of spacetime with a fixed time-flow vector field. For existence of a well-defined Hamiltonian variational principle taking into account a spatial boundary, it is necessary to modify the standard Arnowitt-Deser-Misner Hamiltonian by adding a boundary term whose form depends on the spatial boundary conditions for the gravitational field. The most general mathematically allowed boundary conditions and corresponding boundary terms are shown to be determined by solving a certain equation obtained from the symplectic current pulled back to the hypersurface boundary of the spacetime region. A main result is that we obtain a covariant derivation of Dirichlet, Neumann, and mixed type boundary conditions on

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the gravitational field at a fixed boundary hypersurface, together with the associated Hamiltonian boundary terms. As well, we establish uniqueness of these boundary conditions under certain assumptions motivated by the form of the symplectic current. Our analysis uses a Noether charge method which extends and unifies several results developed in recent literature for General Relativity. As an illustration of the method, we apply it to the Maxwell field equations to derive allowed boundary conditions and boundary terms for existence of a well-defined Hamiltonian variational principle for an electromagnetic field in a fixed spatially bounded region of Minkowski spacetime.

I. INTRODUCTION

The mathematical structure of General Relativity as a Hamiltonian field theory is wellunderstood for asymptotically flat spacetimes. As first shown by Regge and Teitelboim [1], with asymptotic fall-off conditions on the metric, there is a modification of the standard Arnowitt-Deser-Misner (ADM) Hamiltonian [2] whose field equations obtained from the Hamiltonian variational principle yield a 3+1 split of the Einstein equations. The ADM Hamiltonian itself yields the 3+1 Einstein equations only if compact support variations of the metric are used in the variational principle. For metric variations satisfying asymptotic fall-off conditions, the ADM Hamiltonian does not give a well-defined variational principle since its variation produces asymptotic boundary terms that do not vanish. However, the boundary terms can be canceled by the addition of a surface integral term at spatial infinity to the ADM Hamiltonian. The resulting Regge-Teitelboim Hamiltonian yields a well-defined variational principle for the Einstein equations with asymptotic fall-off conditions on the metric. On solutions of the Einstein equations the Hamiltonian reduces to a surface integral expression over spatial infinity, which turns out to yield the physically important ADM definition of total energy, momentum, and angular momentum for asymptotically flat spacetimes. Various modern, covariant formulations of this Hamiltonian structure are known |3-7|.

A natural question to investigate is whether this Hamiltonian structure can be extended to spatially bounded regions of spacetime. An important motivation is astrophysical applications where asymptotically flat boundary conditions are not appropriate, e.g. collapse to a black-hole, mergers of binary stars, or collision of black-holes. Another important application is for numerical solution methods of the Einstein equations. In these situations the spatial boundary is not an actual physical boundary in spacetime, but rather is viewed as a mathematically defined timelike hypersurface whose boundary conditions effectively replace the dynamics of the gravitational field in the exterior region.

In this paper and a sequel [8], we work out the covariant Hamiltonian structure of Gen-

eral Relativity for arbitrary spatially compact regions of spacetime $\Sigma \times \mathbf{R}$ whose spacelike slices possess a closed two-surface boundary $\partial \Sigma$, with a fixed time-flow vector field tangent to the timelike hypersurface boundary $\partial \Sigma \times \mathbf{R}$. Rather than start with given boundary conditions on the metric, we instead seek to determine both the most general surface integral term necessary to be added to the ADM Hamiltonian in covariant form together with the most general corresponding boundary conditions on the metric at $\partial \Sigma$ such that the modified Hamiltonian has well-defined variational derivatives. This would yield the most general mathematically allowed variational principle for the Einstein equations with spatial boundary conditions on the metric. To carry out the analysis we employ the covariant Hamiltonian formalism (referred to as the Noether charge method) developed in Ref. [4,9,10].

The main results are that we find Dirichlet and Neumann type boundary conditions for the metric at a spatial boundary two-surface and obtain the associated Hamiltonian surface integrals. Under some natural assumptions motivated by the symplectic structure arising from the ADM Hamiltonian, the most general allowed boundary conditions are shown to be certain types of mixtures of the Dirichlet and Neumann ones. We also investigate the geometrical structure of the Dirichlet and Neumann covariant Hamiltonians. These each turn out to involve an underlying "energy-momentum" vector at each point in the tangent space of the spacetime at the two-surface. In the Dirichlet case, this vector depends only on the extrinsic geometry of the spatial boundary two-surface. Most strikingly, when the vector is decomposed into tangential and normal parts with respect to the two-surface, the normal part yields a direction in which the two-surface has zero expansion in the spacetime.

In Sec. II we first apply the Noether charge formalism to investigate, as an illustrative example, the covariant Hamiltonian structure of the free Maxwell equations on spatially compact regions of Minkowski spacetime. We show that this analysis leads to Dirichlet and Neumann type boundary conditions on the electromagnetic field, corresponding to conductor and insulator type boundaries, as well as mixed type boundary conditions which are linear combinations of the Dirichlet and Neumann ones. We also investigate more general boundary conditions which give rise to a well-defined Hamiltonian variational principle for the

Maxwell equations, and we obtain a uniqueness result for the mixed and pure type Dirichlet and Neumann boundary conditions under some assumptions. The associated Dirichlet and Neumann Hamiltonians are shown to reduce to expressions for the total energy of the electromagnetic field, including contributions from surface electric charge and current due to the boundary conditions.

In Sec. III we carry out the corresponding analysis of the covariant Hamiltonian structure of General Relativity for arbitrary spatially compact regions of spacetime with a closed two-surface boundary, without matter fields. We make some concluding remarks in Sec. IV. In an Appendix we develop the Noether charge method for general Lagrangian field theories with a time symmetry. This approach extends and unifies some aspects of the covariant Hamiltonian formalism introduced in recent literature [4,9–11]. (Throughout we use the notation and conventions of Ref. [12].)

Inclusion of matter fields and analysis of the geometrical properties of the resulting Dirichlet and Neumann Hamiltonians for General Relativity will be investigated in Ref. [8]. It is also left to that paper to discuss the relation between these Hamiltonians and the Regge-Teitelboim Hamiltonian in the case when the two-surface boundary is taken in a limit to be spatial infinity in an asymptotically flat spacetime.

II. ELECTRODYNAMICS

To illustrate our basic approach and the covariant Hamiltonian (Noether charge) formalism, we consider the free Maxwell field theory in 4-dimensional Minkowski spacetime (R^4, η_{ab}) .

We use the standard electromagnetic field Lagrangian, where the field variable is the electromagnetic potential 1-form A_a , with the field strength 2-form defined as $F_{ab} = \partial_{[a} A_{b]}$. The Lagrangian 4-form for the field A_a is given by

$$L_{abcd}(A) = \frac{1}{2} \epsilon_{abcd} F_{mn} F^{mn} = 3F_{[ab} * F_{cd]}$$
 (2.1)

where $*F_{ab} = \epsilon_{ab}^{\ \ cd} F_{cd}$ is the dual field strength 2-form defined using the volume form ϵ_{abcd} . A variation of this Lagrangian gives

$$\delta L_{abcd}(A) = \partial_{[a}\Theta_{bcd]}(A, \delta A) + 6\delta A_{[a}(\partial_b * F_{cd]})$$
(2.2)

where

$$\Theta_{bcd}(A,\delta A) = 6\delta A_{[b}*F_{cd]} \eqno(2.3)$$

defines the symplectic potential 3-form. From Eq. (2.2), one obtains the field equations

$${\mathcal E}_{bcd}(A) = 6 \partial_{[b} * F_{cd]} = 0, \tag{2.4}$$

or equivalently, after contraction with the volume form,

$$\partial^a F_{ab} = \partial^a \partial_{[a} A_{b]} = 0 (2.5)$$

which is the source-free Maxwell equations for A_a .

Let $\xi^a = (\partial/\partial t)^a$ be a timelike isometry of the Minkowski metric, with unit normalization $\xi^a \xi^b \eta_{ab} = -1$, and let Σ be a region contained in a spacelike hyperplane t = 0 orthogonal to ξ^a with the boundary of the region being a closed 2-surface $\partial \Sigma$. Denote the unit outward spacelike normal to $\partial \Sigma$ in Σ by s^a , and denote the metric and volume form on $\partial \Sigma$ by $\sigma_{ab} = \eta_{ab} - s_a s_b + \xi_a \xi_b$ and $\epsilon_{ab} = \epsilon_{abcd} s^c \xi^d$. Let Σ_t and $\partial \Sigma_t$ be the images of Σ and $\partial \Sigma$ under the one-parameter diffeomorphism generated by ξ^a on Minkowski spacetime. Denote the metric compatible derivative operator on $\partial \Sigma$ by \mathcal{D}_a . Let

$$\mathcal{L}_{\xi}A_{a} = \xi^{e}\partial_{e}A_{a} + A_{e}\partial_{a}\xi^{e} = 2\xi^{e}\partial_{[e}A_{a]} + \partial_{a}(\xi^{e}A_{e}), \tag{2.6}$$

which is the Lie derivative of A_a with respect to $\boldsymbol{\xi}^e$.

The Noether current 3-form associated to ξ^a is given by

$$J_{abc}(\xi, A) = \Theta_{abc}(A, \mathcal{L}_{\xi}A) + 4\xi^{d}L_{abcd}(A) = 6*F_{[bc}\mathcal{L}_{\xi}A_{a]} + 12\xi^{d}F_{[ab}*F_{cd]}, \tag{2.7}$$

which simplifies to

$$J_{abc}(\xi, A) = 6\partial_{[a}(*F_{bc]}\xi^{d}A_{d}) + 2\xi^{e}\epsilon_{abcd}(\delta^{d}_{e}F_{mn}F^{mn} - 4F_{en}F^{dn}) - \xi^{e}A_{e}\mathcal{E}_{abc}(A)$$
 (2.8)

after use of Eqs. (2.4) and (2.6). Hence, one obtains the Noether current on solutions A_a ,

$$J_{abc}(\xi, A) = 6\partial_{[a}(*F_{bc]}\xi^d A_d) + 2\xi^e \epsilon_{abcd}(\delta_e^d F_{mn} F^{mn} - 4F_{en} F^{dn}). \tag{2.9}$$

(Note, one easily sees that this 3-form $J_{abc}(\xi,A)$ is closed but is not exact, i.e. there does not exist a Noether current potential $Q_{bc}(\xi,A)$ satisfying $J_{abc}(\xi,A)=3\partial_{[a}Q_{bc]}(\xi,A)$.) Correspondingly, the Noether charge on solutions A_a is given by

$$Q_{\Sigma}(\xi) = \int_{\Sigma} J_{abc}(\xi; A) = \int_{\Sigma} \epsilon_{abcd} \xi^e (-8F_{en}F^{dn} + 2\delta_e^d F_{mn}F^{mn}) + \oint_{\partial \Sigma} 2*F_{bc} \xi^d A_d. \tag{2.10}$$

This expression simplifies in terms of the electromagnetic stress-energy tensor defined by

$$T_e^{\ d}(F) = 2F_{en}F^{dn} - \frac{1}{2}\delta_e^d F_{mn}F^{mn}. \tag{2.11}$$

Thus,

$$\frac{1}{4}Q_{\Sigma}(\xi) = \int_{\Sigma} \xi^{e} \xi^{d} T_{de}(F) d^{3}x + \oint_{\partial \Sigma} \xi^{a} A_{a} \xi^{d} s^{e} F_{de} dS$$
(2.12)

where d^3x and dS denote the coordinate volume elements on Σ and $\partial\Sigma$ obtained from the volume forms $\epsilon_{abcd}\xi^d$ and ϵ_{bc} , respectively.

A. Covariant Hamiltonian formulation

The symplectic current, defined by the antisymmetrized variation of $\Theta_{bcd}(A, \delta A)$, is given by the 3-form

$$\frac{1}{6}\omega_{bcd}(\delta_1 A, \delta_2 A) = \delta_1 A_{[b}\delta_2 * F_{cd]} - \delta_2 A_{[b}\delta_1 * F_{cd]}. \tag{2.13}$$

Then the presymplectic form on Σ is given by

$$\Omega_{\Sigma}(\delta_1 A, \delta_2 A) = \int_{\Sigma} \omega_{bcd}(\delta_1 A, \delta_2 A). \tag{2.14}$$

A Hamiltonian conjugate to ξ on Σ is a function $H_{\Sigma}(\xi;A) = \int_{\Sigma} \mathcal{H}_{abc}(\xi;A)$ for some locally constructed 3-form $\mathcal{H}_{abc}(\xi;A)$ such that

$$\delta H_{\Sigma}(\xi; A) \equiv H_{\Sigma}'(\xi; A, \delta A) = \Omega_{\Sigma}(\delta A, \mathcal{L}_{\xi} A) \tag{2.15}$$

for arbitrary variations δA_a away from solutions A_a .

From the expression (2.7) for the Noether current, the presymplectic form yields

$$\Omega_{\Sigma}(\delta A, \mathcal{L}_{\xi} A) = \int_{\Sigma} \delta J_{abc}(\xi, A) + 4\xi^{d} \delta A_{[d} \mathcal{E}_{abc]}(A) - \oint_{\partial \Sigma} \xi^{c} \Theta_{abc}(A, \delta A). \tag{2.16}$$

Hence, for compact support variations δA_a away from solutions A_a , the Noether current gives a Hamiltonian (2.15) with $\mathcal{H}_{abc}(\xi;A)=J_{abc}(\xi,A)$, up to an inessential boundary term. The simplified expression (2.8) for $J_{abc}(\xi,A)$ thereby yields the Hamiltonian

$$H(\xi; A) = 4 \int_{\Sigma} \xi^{e} \xi^{d} (T_{de}(F) + A_{e} \partial^{c} F_{cd}) d^{3} x.$$
 (2.17)

On solutions A_a , this Hamiltonian is equal to the total electromagnetic field energy on Σ , $H(\xi;A)=4\int_{\Sigma}\xi^e\xi^dT_{de}(F)d^3x.$

To define a Hamiltonian (2.15) for variations δA_a without compact support, it follows that the term $\xi^c \Theta_{abc}(A, \delta A)$ in Eq. (2.16) needs to be a total variation at the boundary $\partial \Sigma$, i.e. there must exist a locally constructed 3-form $\tilde{B}_{abc}(A)$ such that one has

$$\xi^{c}\Theta_{abc}(A,\delta A)|_{\partial\Sigma} = (\xi^{c}\delta\tilde{B}_{abc}(A) + \partial_{[a}\alpha_{b]}(\xi;A,\delta A))|_{\partial\Sigma}$$
(2.18)

where $\alpha_b(\xi; A, \delta A)$ is a locally constructed 1-form. This equation holds if and only if, by taking an antisymmetrized variation [10], one has

$$\epsilon^{bc} \xi^{a} \omega_{abc}(\delta_{1} A, \delta_{2} A)|_{\partial \Sigma} = \mathcal{D}_{c} \tilde{\beta}^{c}(\xi; \delta_{1} A, \delta_{2} A)|_{\partial \Sigma}$$
(2.19)

where

$$\tilde{\beta}^{c}(\xi; \delta_{1}A, \delta_{2}A) = \epsilon^{cb}\delta_{1}\alpha_{b}(\xi; A, \delta_{2}A) - \epsilon^{cb}\delta_{2}\alpha_{b}(\xi; A, \delta_{1}A) \tag{2.20}$$

is a locally constructed vector, in $T(\partial \Sigma)$, which is skew bilinear in $\delta_1 A, \delta_2 A$. The term involving the symplectic current is given by

$$\epsilon^{bc}\xi^{a}\omega_{abc}(\delta_{1}A,\delta_{2}A) = 8s^{c}h^{de}(\delta_{1}A_{e}\delta_{2}F_{cd} - \delta_{2}A_{e}\delta_{1}F_{cd}) \tag{2.21}$$

with $h_{ab} = \eta_{ab} - s_a s_b = \sigma_{ab} - \xi_a \xi_b$. Given a solution of equation (2.19), one can then determine $\tilde{B}_{abc}(A)$ from equation (2.18) by

$$\epsilon^{ab}\xi^{c}\tilde{B}_{abc}(A) = \epsilon^{ab}(\xi^{c}\Theta_{abc}(A,\delta A) - \partial_{a}\alpha_{b}(\xi;A,\delta A))$$

$$= 8s^{c}h^{de}F_{cd}\delta A_{e} - \mathcal{D}_{a}\tilde{\alpha}^{a}(\xi;A,\delta A)$$
(2.22)

where

$$\tilde{\alpha}^{a}(\xi; A, \delta A) = \epsilon^{ab} \alpha_{b}(\xi; A, \delta A). \tag{2.23}$$

This leads to the following main result.

Proposition 2.1. A Hamiltonian conjugate to ξ^a on Σ exists for variations δA_a with support on $\partial \Sigma$ if and only if

$$8h^{bc}s^{a}(\delta_{1}A_{b}\partial_{[a}\delta_{2}A_{c]} - \delta_{2}A_{b}\partial_{[a}\delta_{1}A_{c]})|_{\partial\Sigma} = \mathcal{D}_{c}\tilde{\beta}^{c}(\xi;\delta_{1}A,\delta_{2}A)$$
(2.24)

for some locally constructed vector $\tilde{\beta}_a(\xi, \delta_1 A, \delta_2 A)$, in $T(\partial \Sigma)$, which is skew bilinear in $\delta_1 A, \delta_2 A$. The solutions of equation (2.24) of the form $\delta \mathcal{F}_a(A)|_{\partial \Sigma} = 0$ give the allowed boundary conditions $\mathcal{F}_a(A)|_{\partial \Sigma}$ for a Hamiltonian formulation of the Maxwell equations in the local spacetime region Σ_t , $t \geq 0$. For each boundary condition, there is a corresponding Hamiltonian given by the Noether charge plus a boundary term

$$H_{\Sigma}(\xi;A) = \int_{\Sigma} J_{abc}(\xi,A) - \oint_{\partial \Sigma} \xi^{a} \tilde{B}_{abc}(A) \equiv H(\xi;A) + H_{B}(\xi;A), \tag{2.25}$$

with

$$H(\xi; A) = 4 \int_{\Sigma} \xi^{e} \xi^{d} (T_{de}(F) + A_{e} \partial^{c} F_{cd}) d^{3} x, \qquad (2.26)$$

$$H_B(\xi; A) = \oint_{\partial \Sigma} \xi^a (4A_a \xi^d s^e F_{de} - \frac{1}{2} \tilde{B}_a(A)) dS, \tag{2.27}$$

where $\tilde{B}_a(A) = \epsilon^{bc} \tilde{B}_{abc}(A)$ is determined from

$$(\xi^a \tilde{B}_a(A) - 8s^c h^{de} F_{cd} \delta A_e)|_{\partial \Sigma} = \mathcal{D}_a \tilde{\alpha}^a(\xi; A, \delta A)|_{\partial \Sigma}$$
(2.28)

with $\tilde{\alpha}^a(\xi; A, \delta A)$ given by Eqs. (2.20) and (2.23). Note, $\tilde{B}_a(A)$ is unique up to addition of an arbitrary covector function of the fixed boundary data $\mathcal{F}_a(A)$.

The results in Proposition 2.1 take a more familiar form when expressed in terms of the electric and magnetic fields on Σ defined by $E_a = 2\xi^b F_{ab}$, $B_a = \xi^b * F_{ab}$, which are vectors in $T(\Sigma)$ (i.e. $\xi^a E_a = \xi^a B_a = 0$). A convenient notation now is to write vectors in $T(\Sigma)$ using an over script \to , and for tensors on M, to denote tangential and normal components with respect to Σ by subscripts \parallel and \bot , and denote components orthogonal to Σ_t by a subscript 0. Then we have

$$\vec{E} = \vec{\partial}A_0 - \partial_0\vec{A}, \quad \vec{B} = \vec{\partial} \times \vec{A}. \tag{2.29}$$

In this notation, the presymplectic form (2.14) and the Hamiltonian (2.25) reduce to the expressions

$$\frac{1}{4}\Omega_{\Sigma}(\delta_{1}A, \delta_{2}A) = \int_{\Sigma} (\delta_{2}\vec{A} \cdot \delta_{1}\vec{E} - \delta_{1}\vec{A} \cdot \delta_{2}\vec{E})d^{3}x$$

$$= \int_{\Sigma} (\delta_{1}\vec{A} \cdot (\partial_{0}\delta_{2}\vec{A} - \vec{\partial}\delta_{2}A_{0}) - \delta_{2}\vec{A} \cdot (\partial_{0}\delta_{1}\vec{A} - \vec{\partial}\delta_{1}A_{0}))d^{3}x$$
(2.30)

and

$$\frac{1}{2}H_{\Sigma}(\xi;A) = \int_{\Sigma} \frac{1}{2}(\vec{E}^2 + \vec{B}^2) + A_0 \vec{\partial} \cdot \vec{E}_{\perp} \ d^3x - \oint_{\partial \Sigma} A_0 E_{\perp} + \frac{1}{4}\tilde{B}_0(A)dS. \tag{2.31}$$

Note that the Hamiltonian field equations obtained from $H_{\Sigma}(\xi; A)$ are given by the variational principle

$$H'_{\Sigma}(\xi; A, \delta A) = \Omega_{\Sigma}(\delta A, \mathcal{L}_{\xi} A)$$
(2.32)

for arbitrary variations $\delta A_a|_{\Sigma}$. These field equations split into dynamical equations and constraint equations, corresponding to a decomposition of A_a into dynamical and non-dynamical components, respectively \vec{A} and A_0 , determined by [4] the degeneracy of the presymplectic form (2.30). In particular, this yields the Gauss-law constraint equation

$$\vec{\partial} \cdot \vec{E} = \Delta A_0 - \partial_0 \vec{\partial} \cdot \vec{A} = 0 \tag{2.33}$$

obtained from $H'_{\Sigma}(\xi; A, \delta A_0) = 0$ through variation of A_0 , and the dynamical Maxwell evolution equation

$$\partial_0 \vec{E} - \vec{\partial} \times \vec{B} = (-\partial_0^2 + \Delta)\vec{A} + \vec{\partial}(\partial_0 A_0 - \vec{\partial} \cdot \vec{A}) = 0$$
 (2.34)

obtained from $H'_{\Sigma}(\xi; A, \delta \vec{A}) = \Omega_{\Sigma}(\delta \vec{A}, \mathcal{L}_{\xi} A)$ through variation of \vec{A} , where $\Delta = \vec{\partial} \cdot \vec{\partial}$ is the Laplacian on Σ . Thus, the Noether charge (covariant Hamiltonian) formalism here is equivalent to the standard canonical formulation [12] of the Maxwell equations.

B. Dirichlet and Neumann Boundary Conditions

Two immediate solutions of the determining equation (2.24) with $\tilde{\beta}^a = 0$ are boundary conditions associated with fixing components of A_a or $F_{bc} = \partial_{[b} A_{c]}$ at $\partial \Sigma_t$ for $t \geq 0$.

Consider

(D)
$$\sigma_b^a \delta A_a |_{\partial \Sigma_t} = 0, \quad \xi^a \delta A_a |_{\partial \Sigma_t} = 0, \quad t \ge 0,$$
 (2.35)

or equivalently $\delta \vec{A}_{\parallel} = \delta A_0 = 0$, for $t \geq 0$, called Dirichlet boundary conditions, i.e.

$$\mathcal{F}_a^{\mathcal{D}}(A) = h_a^{\ b} A_b; \tag{2.36}$$

(N)
$$\sigma_b^a s^c \delta F_{ac}|_{\partial \Sigma_t} = 0, \quad s^a \xi^c \delta F_{ac}|_{\partial \Sigma_t} = 0, \quad t \ge 0,$$
 (2.37)

or equivalently $\vec{\partial}_{\perp} \times \delta \vec{A}_{\parallel} - \vec{\partial}_{\parallel} \times \delta \vec{A}_{\perp} = \vec{\partial}_{\perp} \delta A_0 - \partial_0 \delta \vec{A}_{\perp} = 0$, for $t \geq 0$, called Neumann boundary conditions, i.e.

$$\mathcal{F}_{a}^{N}(A) = h_{a}^{\ b} s^{c} F_{bc}. \tag{2.38}$$

Theorem 2.2. For the boundary conditions (D) or (N), a Hamiltonian conjugate to ξ^a on Σ , evaluated on solutions A_a , is given by

$$\frac{1}{2}H^{D}(\xi;A) = 2\int_{\Sigma} \epsilon_{dabc} (2\xi^{e} F_{en} F^{dn} - \frac{1}{2}\xi^{d} F_{mn} F^{mn}) + 2\oint_{\partial\Sigma} \epsilon_{bc} \xi^{a} A_{a} \xi^{d} s^{e} F_{de}$$
 (2.39)

$$= \frac{1}{2} \int_{\Sigma} \vec{E}^2 + \vec{B}^2 \ d^3x - \oint_{\partial \Sigma} A_0 E_{\perp} \ dS, \tag{2.40}$$

$$\frac{1}{2}H^{\rm N}(\xi;A) = 2\int_{\Sigma} \epsilon_{dabc} (2\xi^{e} F_{en} F^{dn} - \frac{1}{2}\xi^{d} F_{mn} F^{mn}) + 2\oint_{\partial\Sigma} \epsilon_{bc} \sigma^{bd} A_{b} s^{e} F_{de}$$
 (2.41)

$$= \frac{1}{2} \int_{\Sigma} \vec{E}^2 + \vec{B}^2 \ d^3x - \oint_{\partial \Sigma} (\vec{A} \times \vec{B})_{\perp} \ dS. \tag{2.42}$$

Proof:

For (D), one has

$$\epsilon^{bc}\xi^{a}\Theta_{abc}(A,\mathcal{L}_{\xi}A) = 6\epsilon^{bc}\xi^{a}\delta A_{[a}*F_{bc]}$$

$$= 8(\xi^{a}\delta A_{a}\xi^{d}s^{e}F_{de} - \sigma^{ad}\delta A_{a}s^{e}F_{de}) = 0$$
(2.43)

and hence $\tilde{B}_{abc}(A)=0,$ so thus $\xi^a\tilde{B}_a(A)=0.$ For (N), one has

$$\begin{split} \epsilon^{bc}\xi^{a}\Theta_{abc}(A,\mathcal{L}_{\xi}A) &= 6\epsilon^{bc}\xi^{a}(\delta A_{[a}*F_{bc]}) \\ &= 6\epsilon^{bc}\xi^{a}(\delta (A_{[a}*F_{bc]}) - A_{[a}\delta*F_{bc]}) \\ &= \delta(6\epsilon^{bc}\xi^{a}A_{[a}*F_{bc]}) + 8(-\xi^{a}A_{a}\xi^{d}s^{e}\delta F_{de} + A_{a}\sigma^{ad}s^{e}\delta F_{de}) \\ &= \delta(\epsilon^{bc}\xi^{a}\tilde{B}_{abc}) \end{split} \tag{2.44}$$

with $\tilde{B}_{abc}(A) = 6A_{[a}*F_{bc]}$. Thus,

$$\xi^{a}\tilde{B}_{a}(A) = 6\epsilon^{bc}\xi^{a}A_{[a}*F_{bc]} = 8s_{d}A_{e}F^{de}.$$
(2.45)

Note that for both boundary conditions (D) and (N), the surface integral terms in the Hamiltonian take the form

$$H_B(\xi; A) = 4 \oint_{\partial \Sigma} \xi^a P_a(A) dS$$
 (2.46)

where

$$P_a^{\rm D}(A) = A_a \xi^b s^c F_{bc},$$
 (2.47)

$$P_a^{\rm N}(A) = -\xi_a s^d \sigma^{bc} A_b F_{cd}. \tag{2.48}$$

There is simple physical interpretation of the (D) and (N) boundary conditions: (D) involves fixing A_0 and \vec{A}_{\parallel} at $\partial \Sigma_t$ for $t \geq 0$, which means

$$\vec{E}_{\parallel} = \vec{\partial}_{\parallel} A_0 - \partial_0 \vec{A}_{\parallel}, \quad \vec{B}_{\perp} = \vec{\partial}_{\parallel} \times \vec{A}_{\parallel} \tag{2.49}$$

are specified data at the boundary surface (analogous to a conductor) as a function of time. Note, consequently, \vec{E}_{\perp} and \vec{B}_{\parallel} are left free by the boundary condition (D) and therefore are induced data for solutions A_0 , \vec{A} of the Hamiltonian field equations; (N) reverses the role of the induced and fixed data at the boundary surface, so now \vec{E}_{\perp} and \vec{B}_{\parallel} are specified as a function of time (analogous to an insulator), while the induced data for solutions A_0 , \vec{A} of the Hamiltonian field equations are \vec{E}_{\parallel} and \vec{B}_{\perp} . Note the fixed data here are gauge-equivalent to specifying the normal derivative of A_0 and \vec{A}_{\parallel} at $\partial \Sigma_t$ in Σ_t for $t \geq 0$,

$$\vec{E}_{\perp} = \vec{\partial}_{\perp} (A_0 - \partial_0 \chi), \quad \vec{B}_{\parallel} = \vec{\partial}_{\perp} \times (\vec{A}_{\parallel} - \vec{\partial}_{\parallel} \chi), \tag{2.50}$$

where χ is given by $\vec{\partial}_{\perp}\chi = \vec{A}_{\perp}$.

Moreover, the Hamiltonians (2.40) and (2.42) on solutions A_0 , \vec{A} have the interpretation as expressions for the total energy of the electromagnetic fields, with the surface integral parts representing the energy contribution [13] from an effective (fictitious) surface charge density in the case (D), and effective (fictitious) surface current density in the case (N), associated to the specified data at the boundary surface. In particular, effective surface charges and currents arise, respectively, when \vec{E}_{\perp} or \vec{A}_{\parallel} are left free [13] on the boundary surface.

We remark that similar boundary terms arise in the asymptotic case when the boundary surface is taken to be a 2-sphere at spatial infinity on Σ (see Ref. [14]).

C. Determination of allowed boundary conditions

The symplectic current component $\epsilon^{bc}\xi^a\omega_{abc}(\delta_1A,\delta_2A)$ involves only the field variations $h_a{}^b\delta A_b, h_a{}^bs^c\partial_{[b}\delta A_{c]}$. We refer to the components $\sigma_b{}^cA_c, \xi^cA_c, \sigma_b{}^cs^aF_{ac}, \xi^cs^aF_{ac}$, or equivalently $\vec{A}_{\parallel}, A_0, \vec{B}_{\parallel}, \vec{E}_{\perp}$, as symplectic boundary data at $\partial \Sigma$. Hence, in solving the determining equation (2.24) for the allowed boundary conditions on A_a , it is then natural to restrict attention to boundary conditions involving only this data. (Some remarks on more general boundary conditions are made at the end of this section.) To proceed, we suppose that the

possible boundary conditions are linear, homogeneous functions of the symplectic boundary data, with coefficients locally constructed out of the geometrical quantities ξ^a , s^a , σ_{bc} , ϵ_{bc} at the boundary surface. We call this type of boundary condition a *symplectic* boundary condition.

Theorem 2.3. The most general allowed symplectic boundary conditions

$$\mathcal{F}_b(h_c^d A_d, h_c^d s^e F_{de}; \xi^c, s^c, \sigma_{de}, \epsilon_{de}) \tag{2.51}$$

for existence of a Hamiltonian conjugate to ξ^a on Σ are given by

$$\mathcal{F}_{b} = b_{0} \sigma_{b}^{c} A_{c} + a_{0} \sigma_{b}^{c} s^{a} F_{ac} + b_{1} \xi_{b} \xi^{c} A_{c} + a_{1} \xi_{b} \xi^{c} s^{a} F_{ca}, \tag{2.52}$$

or equivalently,

$$\sigma_b^{\ c}(b_0\delta A_c + a_0 s^a \delta F_{ac})|_{\partial \Sigma_t} = 0, \quad t \ge 0, \tag{2.53}$$

$$\xi^{c}(b_{1}\delta A_{c} + a_{1}s^{a}\delta F_{ac})|_{\partial\Sigma_{t}} = 0, \quad t \ge 0$$
(2.54)

for any constants a_0, b_0 (not both zero), a_1, b_1 (not both zero).

Proof:

First, we show that $\tilde{\beta}^a = 0$ without loss of generality in the determining equation (2.24) for boundary conditions of the form (2.51). Note the left side of Eq. (2.24) is algebraic in $\delta A_a, \delta F_{ab} = \partial_{[a} \delta A_{b]}$. Since the right side necessarily involves at least one derivative on δA_a , we must have

$$\tilde{\beta}^a = \delta_1 A_b \delta_2 A_c \beta^{abc} \tag{2.55}$$

for some tensor

$$\beta^{abc} = \sigma_e^{\ a} \beta^{e[bc]}. \tag{2.56}$$

We substitute expression (2.55) into Eq. (2.24) and collect all terms that do not involve just the symplectic boundary data, namely $s^c A_c$, $\xi^c \sigma_d^a F_{ac}$, $\sigma_b^c \sigma_d^a F_{ac}$, and $\partial_{(a} A_{b)}$. The coefficients of these terms yield algebraic equations

$$s_c \beta^{(ab)c} = 0, \quad s_c \beta^{[ab]c} = 0, \quad s^{[d} \beta^{ab]c} = 0.$$
 (2.57)

Then, since β^{abc} has the form (2.56), we find that the solution of the equations in (2.57) is

$$\beta^{abc} = 0 \tag{2.58}$$

and so $\tilde{\beta}^a = 0$.

Hence, the determining equation (2.24) reduces to

$$h^{bc}s^{a}(\delta_{1}A_{b}\partial_{[a}\delta_{2}A_{c]} - \delta_{1}A_{b}\partial_{[a}\delta_{1}A_{c]})|_{\partial\Sigma} = 0, \tag{2.59}$$

which we are now free to solve as a purely algebraic equation in terms of the variables δA_b and $\delta F_{ac} = \partial_{[a} \delta A_{c]}$, i.e.

$$h^{bc}s^{a}(\delta_{1}A_{b}\delta_{2}F_{ac} - \delta_{1}A_{b}\delta_{2}F_{ac}) = 0. {(2.60)}$$

It is straightforward to show from the form of Eq. (2.60) that the only solution which is linear, homogeneous in the previous variables is given by

$$\Pi_{1b}{}^c \delta A_c = \Pi_{2b}{}^c s^a \delta F_{ac} \tag{2.61}$$

where $\Pi_1{}^{bc}$ and $\Pi_2{}^{bc}$ are some symmetric tensors orthogonal to s^a , such that Eq. (2.61) can be solved for either $\xi^b \delta A_b$ or $\xi^b s^a \delta F_{ab}$, and either $\sigma_c{}^b \delta A_b$ or $\sigma_c{}^b s^a \delta F_{ab}$. Since we require the coefficients in the boundary conditions under consideration to be locally constructed out of $\xi^a, s^a, \sigma_{bc}, \epsilon_{bc}$, we see that

$$\Pi_1^{bc} = b_0 \sigma^{bc} + b_1 \xi^b \xi^c, \quad \Pi_2^{bc} = a_0 \sigma^{bc} + a_1 \xi^b \xi^c,$$
 (2.62)

for some constants a_0, a_1, b_0, b_1 with $a_0 \neq 0$ or $b_0 \neq 0$, and $a_1 \neq 0$ or $b_1 \neq 0$. This yields the general solution (2.53) and (2.54) given in the Theorem.

The boundary conditions given by Theorem 2.3 comprise the following separate types: (i) for $a_0 = a_1 = 0$ or $b_0 = b_1 = 0$, one obtains, respectively, Dirichlet (2.35) and Neumann (2.37) boundary conditions; (ii) for $b_0 = 0(a_0 \neq 0)$, $b_1 \neq 0$, the boundary conditions yield a one-parameter $a_1/b_1 \equiv c_1$ family of the form

$$\sigma_b^c s^a \delta F_{ac}|_{\partial \Sigma_t} = 0, \quad \xi^c \delta A_c|_{\partial \Sigma_t} = -c_1 s^a \xi^c \delta F_{ac}|_{\partial \Sigma_t}, \quad t \ge 0, \tag{2.63}$$

or equivalently, $\delta \vec{B}_{\parallel} = \vec{s} \delta A_0 + c_1 \frac{1}{2} \delta \vec{E}_{\perp} = 0$, for $t \geq 0$; (iii) similarly, for $b_1 = 0 (a_1 \neq 0)$, $b_0 \neq 0$, the boundary conditions yield another one-parameter $a_0/b_0 \equiv c_0$ family of the form

$$\sigma_b^c \delta A_c |_{\partial \Sigma_t} = -c_0 s^a \delta F_{ab} |_{\partial \Sigma_t}, \quad \xi^c s^a \delta F_{ac} |_{\partial \Sigma_t} = 0, \quad t \ge 0, \tag{2.64}$$

or equivalently, $\vec{s} \times \delta \vec{A}_{\parallel} + c_0 \frac{1}{2} \delta \vec{B}_{\parallel} = \delta \vec{E}_{\perp} = 0$, for $t \geq 0$; (iv) finally, for $b_0 \neq 0, b_1 \neq 0$ ($a_0 \neq 0, a_1 \neq 0$), we obtain a two-parameter $a_1/b_1 \equiv c_1$ and $a_0/b_0 \equiv c_0$ family of the boundary conditions

$$\sigma_b^c \delta A_c |_{\partial \Sigma_t} = -c_0 s^a \delta F_{ab} |_{\partial \Sigma_t}, \quad \xi^c \delta A_c |_{\partial \Sigma_t} = -c_1 s^a \xi^c \delta F_{ac} |_{\partial \Sigma_t}, \quad t \ge 0, \tag{2.65}$$

or equivalently, $\vec{s} \times \delta \vec{A}_{\parallel} + c_0 \frac{1}{2} \delta \vec{B}_{\parallel} = \vec{s} \delta A_0 + c_1 \frac{1}{2} \delta \vec{E}_{\perp} = 0$, for $t \geq 0$.

The fixed data for these boundary conditions (2.63) to (2.65) corresponds to specifying, respectively, the field components

$$\vec{s}A_0 + c_1 \frac{1}{2} \vec{E}_\perp, \quad \vec{B}_\parallel, \quad c_1 \neq 0,$$
 (2.66)

$$\vec{E}_{\perp}, \quad \vec{s} \times \vec{A}_{\parallel} + c_0 \frac{1}{2} \vec{B}_{\parallel}, \quad c_0 \neq 0,$$
 (2.67)

$$\vec{s}A_0 + c_1 \frac{1}{2}\vec{E}_\perp, \quad \vec{s} \times \vec{A}_{\parallel} + c_0 \frac{1}{2}\vec{B}_{\parallel}, \quad c_0 \neq 0, c_1 \neq 0,$$
 (2.68)

at the boundary surface Σ_t for $t \geq 0$. From Proposition 2.1, we readily obtain the Hamiltonian boundary terms corresponding to these boundary conditions (by a proof similar to that for Theorem 2.2).

Theorem 2.4. For boundary conditions (2.63) to (2.65), there is a respective Hamiltonian (2.25) conjugate to ξ^a on Σ , with boundary terms given by

$$H_{B}(\xi; A) = 4 \oint_{\partial \Sigma} \epsilon_{bc} (\xi^{a} A_{a} \xi^{d} s^{e} F_{de} + \sigma^{ad} A_{a} s^{e} F_{de} - c_{1} (\xi^{d} s^{e} F_{de})^{2})$$

$$= -\oint_{\partial \Sigma} 2(\vec{A} \times \vec{B})_{\perp} + c_{1} \vec{E}_{\perp}^{2} dS, \qquad (2.69)$$

$$H_B(\xi; A) = 4 \oint_{\partial \Sigma} \epsilon_{bc} c_0 \sigma^{de} s^a F_{ad} s^m F_{me}$$

$$= \oint_{\partial \Sigma} c_0 \vec{B}_{\parallel}^2 dS, \qquad (2.70)$$

$$H_{B}(\xi; A) = 4 \oint_{\partial \Sigma} \epsilon_{bc} (\xi^{a} A_{a} \xi^{d} s^{e} F_{de} - c_{1} (\xi^{d} s^{e} F_{de})^{2} + c_{0} \sigma^{de} s^{m} F_{md} s^{n} F_{ne})$$

$$= - \oint_{\partial \Sigma} 2A_{0} \vec{E}_{\perp} + c_{1} E_{\perp}^{2} - c_{0} \vec{B}_{\parallel}^{2} dS.$$
(2.71)

Interestingly, among the allowed boundary conditions given by Theorem 2.3, we observe that the Hamiltonian boundary terms vanish identically in one (and only one) case, when $c_0 = 0$ in boundary condition (2.64), i.e.

$$\sigma_b^c \delta A_c|_{\partial \Sigma_t} = 0, \quad \xi^c s^a \delta F_{ac}|_{\partial \Sigma_t} = 0, \quad t \ge 0,$$
 (2.72)

or equivalently, $\delta \vec{A}_{\parallel} = \delta \vec{E}_{\perp} = 0$, for $t \geq 0$. The resulting Hamiltonian (2.25) reduces, on solutions A_a , simply to the expression for the total energy of the electromagnetic fields, $H(\xi;A) = 4 \int_{\Sigma} \xi^e \xi^d T_{de}(F) d^3x = \int_{\Sigma} \vec{E}^2 + \vec{B}^2 d^3x$. The fixed data corresponding to the boundary condition (2.72) is \vec{A}_{\parallel} and \vec{E}_{\perp} , which means that the normal components of the electric and magnetic fields at $\partial \Sigma$ are specified for $t \geq 0$,

$$\vec{B}_{\perp} = \vec{\partial}_{\parallel} \times \vec{A}_{\parallel}, \quad \vec{E}_{\perp} = \vec{\partial}_{\perp} A_0 - \partial_0 \vec{A}_{\perp}. \tag{2.73}$$

Since \vec{A}_{\parallel} and \vec{E}_{\perp} are fixed, there are no effective charges and currents associated to the boundary surface. Thus, the total electromagnetic energy involves no surface integral contributions in this case.

D. Remarks

We conclude with some short remarks on uniqueness of the boundary conditions obtained in Theorem 2.3.

Note that the symplectic boundary conditions (2.53) and (2.54) are linear combinations of the tangential and normal parts of the Dirichlet and Neumann boundary conditions, referred to as mixed boundary conditions. In physical terms, they correspond to specifying $b_0 \sigma_b^{\ c} A_c + a_0 s^a \sigma_b^{\ c} F_{ac}$ and $b_1 \xi^c A_c + a_1 \xi^c s^a F_{ca}$ as boundary data at $\partial \Sigma_t$ for $t \geq 0$. Theorem 2.3 gives a uniqueness result for these mixed boundary conditions under the natural assumption

(2.51) about the general type of boundary condition considered on the fields at the boundary surface. If this assumption is loosened, then there exist additional boundary conditions allowed by the determining equation (2.24).

In particular, one can trade off some of the mixed boundary conditions on the symplectic boundary data for boundary conditions involving the symmetrized derivatives of A_a at $\partial \Sigma$. For example, an allowed boundary condition satisfying Eq. (2.24) is given by $\mathcal{F}(A) = (\xi^a A_a, \sigma^{ab} \partial_a A_b, \sigma^{ab} s^c \partial_{(b} A_{c)})$, or equivalently

$$\xi^{a}\delta A_{a}|_{\partial\Sigma_{t}} = 0, \quad \sigma^{ab}\partial_{a}\delta A_{b}|_{\partial\Sigma_{t}} = 0, \quad \sigma^{ab}s^{c}\partial_{(b}\delta A_{c)}|_{\partial\Sigma_{t}} = 0, \quad t \geq 0, \tag{2.74}$$

with $\alpha_a = 8\epsilon_a^{\ b}A_b s^c \delta A_c$. From Eq. (2.28) one obtains

$$\frac{1}{8}\xi^a \tilde{B}_a = s^e \sigma^{cd} (A_c \partial_{(d} A_{e)} - A_e \partial_c A_d) - \frac{1}{2} A_d A_e \mathcal{D}^d s^e$$
 (2.75)

where $\mathcal{D}_d s_e = \sigma_d^m \sigma_e^n \partial_m s_n$ is the extrinsic curvature of $\partial \Sigma$ in Σ . Hence the corresponding boundary term in the Hamiltonian is given by Eq. (2.46) with

$$P_{a}(A) = A_{a}s^{d}\xi^{e}F_{de} - s^{e}\sigma^{cd}(A_{c}\partial_{(d}A_{e)} - A_{e}\partial_{c}A_{d}) + \frac{1}{2}A_{d}A_{e}\mathcal{D}^{d}s^{e}.$$
 (2.76)

III. ANALYSIS OF GENERAL RELATIVITY

We now apply the Noether charge analysis to General Relativity, specifically to the vacuum Einstein equations for the gravitational field in a spatially bounded spacetime region with a fixed time-flow vector field. It is straightforward to also include matter fields, as we discuss in Ref. [8].

For General Relativity without matter sources, the starting point is the standard Lagrangian formulation of the Einstein equations with the spacetime metric as the field variable. It turns out, however, that the analysis is considerably simplified by introduction of a tetrad (orthonormal frame). Moreover, taking into account local rotations and boosts of the tetrad, the boundary conditions and resulting Hamiltonians that arise in the tetrad

formulation are equivalent to those obtained purely using the metric formulation, up to a boundary term in the presymplectic form.

After setting up some preliminary notation and results in Sec. III A, we will first consider a Dirichlet boundary condition as explained in Sec. III B. Then we will carry out details of the Noether charge analysis with the Dirichlet boundary condition using the tetrad formulation of General Relativity in Sec. III C. The resulting covariant Dirichlet Hamiltonian for General Relativity is summarized in Sec. III D where we will discuss the equivalence between the metric and tetrad formulations. In Sec. III E we will investigate a Neumann boundary condition and corresponding Hamiltonian, along with more general boundary conditions and Hamiltonians. The main result will be to establish uniqueness of mixed Dirichlet-Neumann boundary conditions for existence of a Hamiltonian formulation of General Relativity. Finally, in Sec. III F we will briefly discuss the form of the Dirichlet and Neumann covariant Hamiltonians, and relate these to an analysis of boundary terms for the ADM Hamiltonian using the standard (non-covariant) ADM canonical variables.

A. Preliminaries

On a given smooth orientable 4-dimensional spacetime manifold M, let g_{ab} be the spacetime metric tensor, $\epsilon_{abcd}(g)$ be the volume form normalized with respect to the metric, and ${}^{g}\nabla_{a}$ be the covariant (torsion-free) derivative operator determined by the metric.

Now, let ξ^a be a complete, smooth timelike vector field on M, and let Σ be a region contained in a spacelike hypersurface with the boundary of the region being a closed orientable 2-surface $\partial \Sigma$. Let s^a denote the unit outward spacelike normal to $\partial \Sigma$ orthogonal to ξ^a , let t^a denote the unit future timelike normal to $\partial \Sigma$ orthogonal to s^a . Denote the metric tensor and volume form on $\partial \Sigma$ by

$$\sigma_{ab} = g_{ab} - s_a s_b + t_a t_b, \tag{3.1}$$

$$\epsilon_{ab} = \epsilon_{abcd}(g)s^c t^d. \tag{3.2}$$

This yields the decompositions

$$g_{ab} = \sigma_{ab} + s_a s_b - t_a t_b, \tag{3.3}$$

$$\epsilon_{abcd}(g) = 12t_{[a}s_b\epsilon_{cd]}.\tag{3.4}$$

Note that one has

$$\xi^{a} = Nt^{a} + N^{a}, \quad N^{a}s_{a} = \xi^{a}s_{a} = 0$$
 (3.5)

for some scalar function N and vector function N^a on $\partial \Sigma$. It is convenient to extend the previous structures off $\partial \Sigma$ as follows. Let \mathcal{V} be the spacetime region foliated by the images of Σ under a one-parameter diffeomorphism on M generated by ξ^a , and let \mathcal{B} be the timelike boundary of \mathcal{V} foliated by the images of $\partial \Sigma$. Fix a time function t which is constant on each of the spacelike slices diffeomorphic to Σ under ξ^a in \mathcal{V} and which is normalized by $\xi^a \partial_a t = 1$, such that t = 0 corresponds to Σ . Then \mathcal{B} is a timelike hypersurface in M whose intersection with spacelike hypersurfaces Σ_t given by t = const in \mathcal{V} consists of spacelike 2-surfaces $\partial \Sigma_t$ diffeomorphic to $\partial \Sigma$. Finally, let s^a , t^a , σ_{ab} , ϵ_{ab} , N, N^a be extended to $\partial \Sigma_t$, and let n_a denote the unit future timelike normal to Σ_t parallel to $\partial_a t$.

Note that, by construction, s_a is hypersurface orthogonal to $\mathcal B$ and hence

$$s_{[c}\partial_b s_{a]} = 0. (3.6)$$

If t_a is expressed as a linear combination of s_a , $\partial_a t$, then since $\partial_a t$ obviously is hypersurface orthogonal to $\partial \Sigma_t$, it follows that

$$s_{[a}t_c\partial_b t_{a]} = 0. (3.7)$$

In addition, note that $s^a \partial_a t$ measures the extent to which Σ_t fails to be orthogonal to \mathcal{B} .

Let $(\mathcal{P}_{\partial\Sigma})_a^b$ and $(\mathcal{P}_t)_a^b$ be coordinate projection operators onto the respective tangent spaces of the 2-surface $\partial\Sigma_t$ and the integral curve of t^a , and let $(\mathcal{P}_{\mathcal{B}})_a^b = (\mathcal{P}_{\partial\Sigma})_a^b + (\mathcal{P}_t)_a^b$, which is the projection operator onto the tangent space of the timelike hypersurface \mathcal{B} . Note that these operators are independent of the spacetime metric, as they involve only the manifold structure of \mathcal{B} and $\partial\Sigma_t$ in local coordinates in M.

Hereafter we work in terms of an orthonormal frame θ_a^{μ} (i.e. tetrad) for g_{ab} on M. The frame components of s^a , t^a , n^a , σ_{ab} , ϵ_{ab} , g_{ab} , $\epsilon_{abcd}(g)$ are given by

$$s^{\mu} = s^{a}\theta^{\mu}_{a}, \ t^{\mu} = t^{a}\theta^{\mu}_{a}, \ n^{\mu} = n^{a}\theta^{\mu}_{a},$$
 (3.8)

$$\sigma^{\mu\nu} = \sigma^{ab}\theta^{\mu}_{a}\theta^{\nu}_{b}, \ \epsilon^{\mu\nu} = \epsilon^{ab}\theta^{\mu}_{a}\theta^{\nu}_{b}, \tag{3.9}$$

$$\eta^{\mu\nu} = g^{ab}\theta^{\mu}_{a}\theta^{\nu}_{b}, \ \epsilon^{\alpha\beta\mu\nu} = \epsilon^{abcd}(g)\theta^{\alpha}_{a}\theta^{\beta}_{b}\theta^{\mu}_{c}\theta^{\nu}_{c}, \tag{3.10}$$

where $\eta^{\mu\nu}=\sigma^{\mu\nu}+s^{\mu}s^{\nu}-t^{\mu}t^{\nu}=diag(-1,1,1,1)$ is the Minkowski frame-metric, with $\sigma^{\mu\nu}=diag(0,0,1,1)$. This leads to an orthonormal frame for the metric σ_{ab} , given by

$$\sigma_a^{\ \mu} = \sigma_a^{\ b} \theta_b^{\mu} \tag{3.11}$$

satisfying

$$s_{\mu}\sigma_{a}^{\ \mu} = t_{\mu}\sigma_{a}^{\ \mu} = 0. \tag{3.12}$$

Let the inverse orthonormal frame for g_{ab} and for σ_{ab} be denoted by

$$\theta^{a}_{\mu} = g^{ab}\theta^{\mu}_{b}, \ \sigma^{\ a}_{\mu} = \sigma^{ab}\sigma^{\ \mu}_{b}.$$
 (3.13)

Then, one has the decompositions

$$\theta_a^{\mu} = \sigma_a^{\ \mu} + s_a s^{\mu} - t_a t^{\mu}, \quad \theta_u^a = \sigma_u^{\ a} + s^a s_{\mu} - t^a t_{\mu}. \tag{3.14}$$

For later use, we will partially fix the SO(3,1) local gauge freedom in θ_{μ}^{a} by choosing the coefficients s_{μ} , t_{μ} in the frame decomposition (3.14) to be fixed functions on M, so that under a variation δg_{ab} ,

$$\delta s_{\mu} = \delta t_{\mu} = \delta \sigma_{\mu\nu} = 0 \tag{3.15}$$

and hence, correspondingly,

$$\delta s_a = s_\mu \delta \theta_a^\mu, \ \delta t_a = t_\mu \delta \theta_a^\mu, \eqno(3.16)$$

$$\delta\sigma_{ab} = 2\sigma_{\mu\nu}\theta^{\mu}_{(a}\delta\theta^{\nu}_{b)} = 2\sigma_{(a}{}^{\mu}\delta\sigma_{b)\mu}. \tag{3.17}$$

Similarly, one then also has

$$\delta \epsilon_{abcd}(\theta) = 4 \epsilon_{\alpha\beta\mu\nu} \theta^{\alpha}_{[a} \theta^{\beta}_{b} \theta^{\mu}_{c} \delta \theta^{\nu}_{d]} = \epsilon_{abcd}(\theta) \theta^{c}_{\mu} \delta \theta^{\mu}_{c}, \tag{3.18}$$

$$\delta\epsilon_{ab} = 2\epsilon_{\mu\nu}\theta^{\mu}_{[a}\delta\theta^{\nu}_{b]} = \epsilon_{ab}\sigma_{\mu}^{c}\delta\sigma_{c}^{\mu}, \tag{3.19}$$

and thus

$$\delta \epsilon_{\mu\nu} = \delta \epsilon_{\alpha\beta\mu\nu} = 0. \tag{3.20}$$

Consequently, some useful identities are given by

$$\delta\theta_a^{\mu} = \delta\sigma_a^{\ \mu} + s^{\mu}\delta s_a - t^{\mu}\delta t_a,\tag{3.21}$$

$$\delta\theta^a_\mu = -\theta^a_\nu \theta^c_\mu \delta\theta^\nu_c = \delta\sigma^a_\mu + s_\mu \delta s^a - t_\mu \delta t^a. \tag{3.22}$$

Now, a variation of the spacetime metric δg_{ab} can be decomposed into the parts

$$\delta g_{ab} = \delta \sigma_{ab} + 2s_{(a}\delta s_{b)} - 2t_{(a}\delta t_{b)}. \tag{3.23}$$

By hypersurface orthogonality, one has the identities

$$\delta s_a = s_a s^b \delta s_b, \quad \delta t_a = s_a s^b \delta t_b - t_a t^b \delta t_b \tag{3.24}$$

and

$$\delta\sigma_{ab} = \sigma_a^c \sigma_b^d \delta\sigma_{cd} + \sigma_a^c s_b s^d \delta\sigma_{cd} - \sigma_a^c t_b t^d \delta\sigma_{cd}. \tag{3.25}$$

Then, from the relation

$$\delta g^{ab} = \delta \sigma^{ab} + 2s^{(a}\delta s^{b)} - 2t^{(a}\delta t^{b)} = -g^{ac}g^{bd}\delta g_{cd}, \tag{3.26}$$

it straightforwardly follows that

$$\delta \sigma^{ab} = -\sigma^{ac} \sigma^{bd} \delta \sigma_{cd}, \tag{3.27}$$

$$\delta s^a = \sigma_b^{\ a} \delta s^b + s^a s_b \delta s^b - t^a t_b \delta s^b, \tag{3.28}$$

$$\delta t^a = \sigma_b^a \delta t^b - t^a t_b \delta t^b, \tag{3.29}$$

where

$$\sigma_{ab}\delta s^b = -s^b \delta \sigma_{ab}, \ \sigma_{ab}\delta t^b = -t^b \delta \sigma_{ab}, \tag{3.30}$$

$$s_b \delta s^b = -s^b \delta s_b, \ t_b \delta s^b = -t^b \delta s_b, \ t_b \delta t^b = -t^b \delta t_b, \tag{3.31}$$

and again by hypersurface orthogonality,

$$s_a \delta \sigma^{ab} = t_a \delta \sigma^{ab} = 0, \quad s_a \delta t^a = 0. \tag{3.32}$$

Thus, the linearly independent parts of $\delta\theta_a^\mu$, or equivalently of $\delta\theta_\mu^a$, are given by

$$\delta \sigma_{\mu}^{a}, \sigma_{b}^{a} \delta s^{b}, \ \sigma_{b}^{a} \delta t^{b}, \ s_{b} \delta s^{b}, \ t_{b} \delta s^{b}, \ t_{b} \delta t^{b}. \tag{3.33}$$

Throughout, the time-flow vector field ξ^a is taken to be fixed, $\delta \xi^a = 0$, under variations of θ_a^{μ} .

B. Dirichlet boundary condition

There is a natural motivation for a Dirichlet boundary condition on the gravitational field in the Einstein equations in analogy with the Maxwell equations where the tangential components of the electromagnetic field potential A_a are specified at the boundary. For General Relativity, similarly, one can introduce a Dirichlet boundary condition given by specifying the tangential components of the spacetime metric g_{ab} at the 2-surfaces $\partial \Sigma_t$. This boundary condition is expressed equivalently by conditions on the variation of the metric tensor

$$\delta \sigma_{ab}|_{\partial \Sigma_t} = 0, \quad \delta t_a|_{\partial \Sigma_t} = 0, \quad t \ge 0.$$
 (3.34)

Geometrically, this means that the metric given by

$$h_{ab} = \sigma_{ab} - t_a t_b \tag{3.35}$$

on the timelike boundary hypersurface \mathcal{B} is specified data, so it is held fixed under variations of g_{ab} ,

$$\delta h_{ab} = 0 \quad \text{on } \mathcal{B}. \tag{3.36}$$

The geometrical form (3.36) of the Dirichlet boundary condition is often introduced when one considers an action principle for General Relativity on a spacetime manifold with a fixed global timelike boundary hypersurface [12,15–17]. We will see in the next section that this boundary condition in the form (3.34) emerges naturally from the Noether charge analysis for the existence of a Hamiltonian formulation of General Relativity for a spatially bounded local spacetime region.

Note that, from the relations (3.27) to (3.31), one can decompose the Dirichlet boundary condition (3.34) into an intrinsic part

$$\delta h^{ab}|_{\partial \Sigma_t} = -h^{ac} h^{bd} \delta h_{cd}|_{\partial \Sigma_t} = 0, \quad t \ge 0$$
(3.37)

and an extrinsic part

$$h_{ab}\delta s^b|_{\partial \Sigma_t} = -s^b \delta h_{ab}|_{\partial \Sigma_t} = 0, \quad t \ge 0$$
(3.38)

with respect to the timelike hypersurface \mathcal{B} . The intrinsic part corresponds to fixing just the metric $\mathcal{P}_{\mathcal{B}}h_{ab}$ restricted to the tangent space of \mathcal{B} , where the projection $\mathcal{P}_{\mathcal{B}}$ removes components of the hypersurface metric proportional to s_a . Correspondingly, note that the volume form

$$\epsilon_{abc}(h) = \epsilon_{abcd}(g)s^d = 3\epsilon_{[ab}t_{c]} \tag{3.39}$$

on this surface is also fixed, $\delta \epsilon_{abc}(h) = 0$ on \mathcal{B} , since

$$\delta \epsilon_{abc}(h) = \frac{1}{2} \epsilon_{abc}(h) h^{mn} \delta h_{mn} = -\frac{1}{2} \epsilon_{abc}(h) h_{mn} \delta h^{mn}. \tag{3.40}$$

The Dirichlet boundary condition has a simple formulation in terms of the orthonormal frame θ_a^{μ} . It is convenient to introduce a frame for the metric h_{ab} by

$$h_a^{\ \mu} = h_a^{\ b} \theta_b^{\mu} = \sigma_a^{\ \mu} - t_a t^{\mu}, \tag{3.41}$$

and inverse frame

$$h^{a\mu} = h^{ab}h_b^{\ \mu}. \tag{3.42}$$

Then the Dirichlet boundary condition (3.34) is equivalent to

$$\delta h_a^{\mu}|_{\partial \Sigma_t} = 0, \quad t \ge 0, \tag{3.43}$$

with intrinsic part

$$\delta h^{a\mu}|_{\partial \Sigma_t} = 0, \quad t \ge 0, \tag{3.44}$$

which is equivalent to Eq. (3.37). These equivalences are immediate consequences of the identities $h_{ab} = h_a^{\ \mu} h_b^{\ \nu} \eta_{\mu\nu}$ and $h^{ab} = h_\mu^{\ a} h_\nu^{\ b} \eta^{\mu\nu}$. From these identities, one also has

$$\delta h_{ab} = 2h_{(a}^{\mu} \delta h_{b)\mu}, \tag{3.45}$$

$$\delta \epsilon_{abc}(h) = h_{\mu}^{\ d} \delta h_{d}^{\ \mu}. \tag{3.46}$$

An additional useful identity is given by

$$\delta h_a^c = -(s^c \delta s_a + s_a \delta s^c) = -s_a h_b^c \delta s^b \tag{3.47}$$

and therefore $\mathcal{P}_{\mathcal{B}}\delta h_a^{\ c}=0$.

Finally, note that the intrinsic part of the Dirichlet boundary condition on the frame decomposes into

$$\delta \sigma^{a\mu}|_{\partial \Sigma_t} = 0, \quad \delta t^a|_{\partial \Sigma_t} = 0, \quad t \ge 0.$$
 (3.48)

The full, extrinsic Dirichlet boundary condition is necessary and sufficient for $\delta h_a^{\ c}|_{\partial \Sigma_t} = 0, t \geq 0.$

C. Noether charge analysis

We consider the standard tetrad formulation of General Relativity, using an orthonormal frame θ^{μ}_a for g_{ab} and a frame-connection

$$\Gamma_a^{\ \mu\nu}(\theta) = \theta^{b\mu g} \nabla_a \theta_b^{\nu} = 2\theta^{b[\mu} \partial_{[a} \theta_{b]}^{\nu]} - \theta^{b\mu} \theta^{c\nu} \theta_{a\alpha} \partial_{[b} \theta_{c]}^{\alpha}. \tag{3.49}$$

Here the expression in the second equality is obtained from the relation

$$\theta_{[b}^{\nu}\Gamma_{a]\nu}^{\ \mu}(\theta) = {}^{g}\nabla_{[a}\theta_{b]}^{\nu} = \partial_{[a}\theta_{b]}^{\mu}.$$
 (3.50)

The curvature of this connection (3.49) is given by

$$R_{ab}^{\ \mu\nu}(\theta) = 2\partial_{[a}\Gamma_{b]}^{\ \mu\nu}(\theta) + 2\Gamma_{[a}^{\ \mu\sigma}(\theta)\Gamma_{b]\sigma}^{\ \nu}(\theta) = R_{abcd}(g)\theta^{c\mu}\theta^{d\nu}, \tag{3.51}$$

related to the Riemann curvature tensor $R_{abcd}(g)$ of g_{ab} .

With θ_a^{μ} as the field variable, the Lagrangian 4-form for General Relativity (without matter sources) is given by

$$L_{abcd}(\theta) = \epsilon_{abcd}(\theta)R(\theta) = 6\theta^{\mu}_{[a}\theta^{\nu}_{b}\tilde{R}_{cd]\mu\nu}(\theta)$$
(3.52)

where

$$\tilde{R}_{cd}^{\ \mu\nu}(\theta) = R_{cd\alpha\beta}(\theta)\epsilon^{\alpha\beta\mu\nu} = 2\partial_{[a}\tilde{\Gamma}_{b]}^{\ \mu\nu} - \Gamma_{[a}^{\ \sigma[\mu}(\theta)\tilde{\Gamma}_{b]\sigma}^{\ \nu]}(\theta)$$
(3.53)

in terms of $\tilde{\Gamma}_{a\mu\nu}(\theta) = \Gamma_a^{\ \alpha\beta}(\theta)\epsilon_{\alpha\beta\mu\nu}$. Then the variation of $L_{abcd}(\theta)$ gives, after integration by parts and use of the connection equation (3.50),

$$\frac{1}{6}\delta L_{abcd}(\theta) = 2\delta\theta^{\mu}_{[a}(\theta^{\nu}_{b}\tilde{R}_{cd]\mu\nu}(\theta)) + \frac{1}{6}\partial_{[a}\Theta_{bcd]}(\theta,\delta\theta) \tag{3.54}$$

where

$$\Theta_{bcd}(\theta, \delta\theta) = 12\theta^{\mu}_{[c}\theta^{\nu}_{d}\delta\tilde{\Gamma}_{b]\mu\nu}(\theta) = 8\epsilon_{ebcd}\theta^{\alpha}_{e}\theta^{a}_{\beta}\delta\Gamma_{a}^{\ \alpha\beta}(\theta)$$
(3.55)

defines the symplectic potential 3-form. The field equations for θ_a^{μ} , obtained from the coefficient of $\delta\theta_a^{\mu}$ in Eq. (3.54), are given by

$$\mathcal{E}^{\mu}_{bcd}(\theta) = 12\theta^{\nu}_{[b}\tilde{R}_{cd]\mu\nu}(\theta) = 8\epsilon_{bcda}(\theta)(R^{a\mu}(\theta) - \frac{1}{2}\theta^{a\mu}R(\theta)) = 0. \tag{3.56}$$

Thus θ_a^{μ} satisfies $R^{a\mu}(\theta) = 0$, which is equivalent to the vacuum Einstein equations for the spacetime metric

$$R_{ab}(g) = 0 (3.57)$$

arising as the stationary points of the action functional $S(g) = \int_M \epsilon_{abcd}(g) R(g)$ under compact support variations of g_{ab} .

The Noether current associated to ξ^a is given by the 3-form

$$\begin{split} J_{abc}(\xi,\theta) &= \Theta_{abc}(\theta, \mathcal{L}_{\xi}\theta) + 4\xi^{d}L_{abcd}(\theta) \\ &= 12\theta^{\mu}_{[b}\theta^{\nu}_{c}\mathcal{L}_{\xi}\tilde{\Gamma}_{a]\mu\nu}(\theta) + 24\xi^{d}\theta^{\mu}_{[c}\theta^{\nu}_{d}\tilde{R}_{ab]\mu\nu}(\theta) \end{split} \tag{3.58}$$

with the first term obtained from the variation of the frame connection (3.49) after replacement of $\delta\theta_a^{\mu}$ by the Lie derivative $\mathcal{L}_{\xi}\theta_a^{\mu} = \xi^e\partial_e\theta_a^{\mu} + \theta_e^{\mu}\partial_a\xi^e$ and use of the fact that Lie derivatives commute with exterior (skew) derivatives. We now simplify the first term in Eq. (3.58) as follows. First we express

$$\mathcal{L}_{\xi}\Gamma_{a}^{\ \mu\nu}(\theta) = \partial_{a}(\xi^{e}\Gamma_{e}^{\ \mu\nu}(\theta)) + \xi^{e}(R_{ea}^{\ \mu\nu}(\theta) - 2\Gamma_{[e}^{\ \mu\sigma}(\theta)\Gamma_{a]\sigma}^{\ \nu}(\theta)). \tag{3.59}$$

Hence we obtain

$$12\theta^{\mu}_{[b}\theta^{\nu}_{c}\mathcal{L}_{\xi}\tilde{\Gamma}_{a]\mu\nu}(\theta) = \partial_{[a}(12\theta^{\mu}_{b}\theta^{\nu}_{c}\xi^{e}\tilde{\Gamma}_{e\mu\nu}(\theta)) - 12\xi^{e}\theta^{\mu}_{[b}\theta^{\nu}_{c}\tilde{R}_{a]e\mu\nu}(\theta)$$

$$(3.60)$$

through use of the identity (3.53). Next we combine the second terms in both Eqs. (3.58) and (3.60) to get

$$-12\xi^{e}\theta^{\mu}_{[b}\theta^{\nu}_{c}\tilde{R}_{a]e\mu\nu}(\theta) + 24\xi^{d}\theta^{\mu}_{[c}\theta^{\nu}_{d}\tilde{R}_{ab]\mu\nu}(\theta) = \xi^{e}\epsilon_{abcd}(g)(4\delta^{d}_{e}R(g) - 8R^{d}_{e}(g)). \tag{3.61}$$

Thus, one obtains the Noether current

$$J_{abc}(\xi;\theta) = 3\partial_{[a}Q_{bc]}(\xi;\theta) - \xi^e \theta_{e\mu} \mathcal{E}^{\mu}_{abc}(\theta)$$
(3.62)

where

$$Q_{bc}(\xi;\theta) = 4\xi^{d}\tilde{\Gamma}_{d\mu\nu}(\theta)\theta_{b}^{\mu}\theta_{c}^{\nu} \tag{3.63}$$

is the Noether current potential 2-form.

On vacuum solutions θ_a^{μ} , the Noether current reduces to an exact 3-form

$$J_{abc}(\xi;\theta) = 3\partial_{[a}Q_{bc]}(\xi;\theta). \tag{3.64}$$

Therefore, the Noether charge for vacuum solutions is given by the boundary 2-surface integral

$$Q_{\Sigma}(\xi) = \int_{\Sigma} J_{abc}(\xi; \theta) = \int_{\partial \Sigma} \epsilon_{bc} 4\xi^{d} \tilde{\Gamma}_{d\mu\nu}(\theta) \epsilon^{\mu\nu} = \int_{\partial \Sigma} 8\xi^{d} \Gamma_{d\mu\nu}(\theta) t^{\mu} s^{\nu} dS$$
 (3.65)

where dS is the volume element on $\partial \Sigma$ corresponding to the volume form ϵ_{bc} in local coordinates.

Now the symplectic current, defined by the antisymmetrized variation of $\Theta_{bcd}(\theta, \delta\theta)$, is given by the 3-form

$$\frac{1}{24}\omega_{bcd}(\theta, \delta_1\theta, \delta_2\theta) = \theta^{\mu}_{[c}\delta_1\theta^{\nu}_d\delta_2\tilde{\Gamma}_{b]\mu\nu}(\theta) - \theta^{\mu}_{[c}\delta_2\theta^{\nu}_d\delta_1\tilde{\Gamma}_{b]\mu\nu}(\theta). \tag{3.66}$$

Then the presymplectic form on Σ is defined by

$$\Omega_{\Sigma}(\theta, \delta_1 \theta, \delta_2 \theta) = \int_{\Sigma} \omega_{bcd}(\theta, \delta_1 \theta, \delta_2 \theta) = 24 \int_{\Sigma} \theta_{[c}^{\mu} \delta_1 \theta_d^{\nu} \delta_2 \tilde{\Gamma}_{b]\mu\nu}(\theta) - \theta_{[c}^{\mu} \delta_2 \theta_d^{\nu} \delta_1 \tilde{\Gamma}_{b]\mu\nu}(\theta). \quad (3.67)$$

A Hamiltonian conjugate to ξ on Σ is a function $H_{\Sigma}(\xi;\theta) = \int_{\Sigma} \mathcal{H}_{abc}(\xi;\theta)$ for some locally constructed 3-form $\mathcal{H}_{abc}(\xi;\theta)$ such that

$$\delta H_{\Sigma}(\xi;\theta) \equiv H_{\Sigma}'(\xi;\theta,\delta\theta) = \Omega_{\Sigma}(\delta\theta,\mathcal{L}_{\xi}\theta) \tag{3.68}$$

holds for arbitrary variations $\delta\theta_a^{\mu}$ away from vacuum solutions θ_a^{μ} .

In terms of the Noether current (3.62), the presymplectic form on Σ yields

$$\Omega_{\Sigma}(\theta, \delta\theta, \mathcal{L}_{\xi}\theta) = \int_{\Sigma} \delta J_{abc}(\xi; \theta) - 4\xi^{d} \mathcal{E}^{\mu}_{[abc}(\theta) \delta\theta_{d]\mu} - \int_{\partial \Sigma} \xi^{c} \Theta_{abc}(\theta, \delta\theta). \tag{3.69}$$

Consequently, for variations $\delta\theta_a^{\mu}$ with compact support on the interior of Σ , the Noether current defines a Hamiltonian conjugate to ξ^a ,

$$H(\xi;\theta) = \int_{\Sigma} J_{abc}(\xi;\theta) = 8 \int_{\Sigma} \xi^{e} \theta_{e\mu} \mathcal{E}^{\mu}_{abc}(\theta) + \int_{\partial \Sigma} Q_{ab}(\xi;\theta), \tag{3.70}$$

which is equal to the Noether charge (3.65) when θ_a^{μ} is a vacuum solution. Explicitly, from Eqs. (3.56) and (3.63), one has

$$H(\xi;\theta) = 8 \int_{\Sigma} \epsilon_{dabc} (\xi^{e} \theta_{\mu}^{d} R_{e}^{\mu}(\theta) - \frac{1}{2} \xi^{d} R(\theta)) + 4 \int_{\partial \Sigma} \epsilon_{bc} \xi^{d} \tilde{\Gamma}_{d\mu\nu}(\theta) \epsilon^{\mu\nu}$$

$$= 8 \int_{\Sigma} \xi^{e} n_{\mu} (R_{e}^{\mu}(\theta) - \frac{1}{2} \theta_{e}^{\mu} R(\theta)) d\Sigma + 8 \int_{\partial \Sigma} \xi^{d} \Gamma_{d\mu\nu}(\theta) t^{\mu} s^{\nu} dS$$
(3.71)

where $d\Sigma$ is the coordinate volume element on Σ obtained from the volume form $\epsilon_{abcd}n^d$.

To define a Hamiltonian $H_{\Sigma}(\xi;\theta)$ for variations $\delta\theta_a^{\mu}$ without compact support, it follows that the term $\xi^c\Theta_{abc}(\theta,\delta\theta)$ in Eq. (3.69) needs to be a total variation at the boundary $\partial\Sigma$, i.e. there must exist a locally constructed 3-form $\tilde{B}_{abc}(\theta)$ such that one has

$$\xi^{c} \Theta_{abc}(\theta, \delta\theta)|_{\partial \Sigma} = (\xi^{c} \delta \tilde{B}_{abc}(\theta) + \partial_{[a} \alpha_{b]}(\xi; \theta, \delta\theta))|_{\partial \Sigma}$$
(3.72)

where $\alpha_b(\xi;\theta,\delta\theta)$ is a locally constructed 1-form. This equation is equivalent to

$$\epsilon^{ab}\xi^{c}\Theta_{abc}(\theta,\delta\theta)|_{\partial\Sigma} = \epsilon^{ab}\xi^{c}\delta\tilde{B}_{abc}(\theta,\delta\theta)|_{\partial\Sigma} + \sigma_{c}^{d}\partial_{d}\tilde{\alpha}^{c}(\xi;\theta,\delta\theta)|_{\partial\Sigma}$$
(3.73)

where $\tilde{\alpha}^c(\xi;\theta,\delta\theta) = \epsilon^{cb}\alpha_b(\xi;\theta,\delta\theta)$ and the symplectic potential term is given by, using identity (3.4),

$$\epsilon^{ab}\xi^{c}\Theta_{abc}(\theta,\delta\theta) = 32\xi^{c}t_{[\alpha}s_{\nu]}\theta^{\alpha}_{c}\theta^{a}_{\mu}\delta\Gamma_{a}^{\mu\nu}(\theta). \tag{3.74}$$

Hence we now have the following result.

Proposition 3.1. A Hamiltonian conjugate to ξ^a on Σ exists for variations $\delta\theta^{\mu}_a$ with support on $\partial\Sigma$ if and only if

$$\epsilon^{ab}\xi^{c}\delta\tilde{B}_{abc}(\theta)|_{\partial\Sigma} = 32(\xi^{c}t_{[\alpha}s_{\nu]}\theta_{c}^{\alpha}\theta_{\mu}^{a}\delta\Gamma_{a}^{\ \mu\nu}(\theta))|_{\partial\Sigma} - \sigma_{c}^{\ d}\partial_{d}\tilde{\alpha}^{c}(\xi;\theta,\delta\theta)|_{\partial\Sigma}$$
(3.75)

for some locally constructed 3-form $\tilde{B}_{abc}(\theta)$ in $T^*(\Sigma)$ and locally constructed vector $\tilde{\alpha}^c(\xi;\theta,\delta\theta)$ in $T(\partial\Sigma)$. The Hamiltonian is given by the Noether charge plus an additional boundary term

$$\begin{split} H_{\Sigma}(\xi;\theta) &= \int_{\Sigma} J_{abc}(\xi;\theta) - \int_{\partial \Sigma} \xi^{c} \tilde{B}_{abc}(\theta) \\ &= 8 \int_{\Sigma} \xi^{e} \theta_{e\mu} \mathcal{E}^{\mu}_{abc}(\theta) + \int_{\partial \Sigma} Q_{ab}(\xi;\theta) - \xi^{c} \tilde{B}_{abc}(\theta) \\ &= 8 \int_{\Sigma} \xi^{e} n_{\mu} (R_{e}^{\ \mu}(\theta) - \frac{1}{2} \theta_{e}^{\mu} R(\theta)) d\Sigma + \int_{\partial \Sigma} \xi^{d} (8 \Gamma_{d\mu\nu}(\theta) t^{\mu} s^{\nu} - \frac{1}{2} \tilde{B}_{d}(\theta)) dS \end{split}$$
(3.76)

 $\label{eq:with Bd} \mbox{with } \tilde{B}_{d}(\theta) = \epsilon^{bc} \tilde{B}_{bcd}(\theta).$

We now show that the equation (3.75) for existence of a Hamiltonian (3.76) is satisfied for the intrinsic Dirichlet boundary condition on θ_a^{μ} ,

$$\delta h^{a\mu}|_{\partial \Sigma_t} = 0, \quad t \ge 0, \tag{3.77}$$

and then we derive the corresponding Hamiltonian boundary term. Henceforth we take θ_a^{μ} to satisfy the gauge conditions (3.15) to (3.17) naturally associated to the boundary hypersurface \mathcal{B} .

Consider the left-side of Eq. (3.75). The boundary condition (3.77) yields $\delta \sigma^{a\mu}|_{\partial \Sigma} = 0$ and hence, from Eq. (3.19), $\delta \epsilon^{ab} = \epsilon^{ab} \sigma_{c\mu} \delta \sigma^{c\mu}|_{\partial \Sigma} = 0$. Thus, we have

$$\epsilon^{ab}\xi^{c}\delta\tilde{B}_{abc}(\theta)|_{\partial\Sigma} = \delta(\epsilon^{ab}\xi^{c}\tilde{B}_{abc}(\theta))|_{\partial\Sigma}. \tag{3.78}$$

Next consider the right-side of Eq. (3.75). We integrate by parts with respect to the variation in the first term to get

$$\xi^{c}t_{[\alpha}s_{\nu]}\theta^{\alpha}_{c}\theta^{a}_{\mu}\delta\Gamma_{a}^{\mu\nu}(\theta) = \delta(\xi^{c}t_{[\alpha}s_{\nu]}\theta^{\alpha}_{c}\theta^{a}_{\mu}\Gamma_{a}^{\mu\nu}(\theta)) - \xi^{c}t_{[\alpha}s_{\nu]}\Gamma_{a}^{\mu\nu}(\theta)(\theta^{a}_{\mu}\delta\theta^{\alpha}_{c} + \theta^{\alpha}_{c}\delta\theta^{a}_{\mu}). \tag{3.79}$$

Then, using orthogonality relations (3.5) and (3.24), we find that the second term in Eq. (3.79) vanishes as follows. First,

$$\xi^c t_{[\alpha} s_{\nu]} \delta \theta_c^{\alpha} = \frac{1}{2} \xi^c (s_{\nu} \delta t_c - t_{\nu} \delta s_c) = -s_{\nu} \xi^c t_c t_b \delta t^b = 0$$

$$(3.80)$$

since $\delta t^b|_{\partial\Sigma} = 0$ by the boundary condition (3.77). In addition,

$$\xi^{c} t_{[\alpha} s_{\nu]} \theta_{c}^{\alpha} \delta \theta_{\mu}^{a} = \frac{1}{2} \xi^{c} t_{c} s_{\nu} (\delta h_{\mu}^{a} + s_{\mu} \delta s^{a}) = -\frac{1}{2} N s_{\nu} s_{\mu} \delta s^{a}. \tag{3.81}$$

Hence, the second term in Eq. (3.79) reduces to

$$\frac{1}{2}Ns_{\nu}s_{\mu}\Gamma_{a}^{\ \mu\nu}(\theta)\delta s^{a}=0 \tag{3.82}$$

since $\Gamma_a^{(\mu\nu)}(\theta) = 0$.

Consequently, returning to equation (3.75), we obtain

$$\delta(\xi^c \tilde{B}_c(\theta) - 32t_{[\alpha} s_{\nu]} \xi^c \theta_c^{\alpha} \theta_{\mu}^a \Gamma_a^{\mu\nu}(\theta))|_{\partial \Sigma} = -\sigma_c^{\ d} \partial_d \tilde{\alpha}^c(\xi; \theta, \delta\theta)|_{\partial \Sigma}$$
(3.83)

which obviously is satisfied by

$$\xi^{c}\tilde{B}_{c}(\theta) = 32t_{[\alpha}s_{\nu]}\xi^{c}\theta^{\alpha}_{c}\theta^{d}_{\mu}\Gamma^{\ \mu\nu}_{d}(\theta) \tag{3.84}$$

and $\tilde{\alpha}^c(\xi;\theta,\delta\theta)=0$. This verifies Proposition 3.1 using the intrinsic Dirichlet boundary condition (3.77).

Finally, from expressions (3.84) for $\xi^c \tilde{B}_c(\theta)$ and (3.63) for $Q_{bc}(\xi,\theta)$, we obtain a Hamiltonian (3.76) with the boundary term given by

$$H_B(\xi,\theta) = \int_{\partial \Sigma} Q_{ab}(\xi,\theta) - \xi^c \tilde{B}_{abc}(\theta,\delta\theta)$$

$$= 8 \int_{\partial \Sigma} \epsilon_{ab} \xi^c (t_{\mu} s_{\nu} \Gamma_c^{\mu\nu}(\theta) - 2t_{[\alpha} s_{\nu]} \theta_c^{\alpha} \theta_{\mu}^d \Gamma_d^{\mu\nu}(\theta)). \tag{3.85}$$

Hence, the Hamiltonian boundary term takes the form

$$H_B(\xi,\theta) = 8 \int_{\partial \Sigma} \xi^c P_c(\theta) dS \tag{3.86}$$

where $P_c(\theta) = t_\mu s_\nu \Gamma_c^{\mu\nu}(\theta) - t_c s_\nu \theta_\mu^a \Gamma_a^{\mu\nu}(\theta) + s_c t_\nu \theta_\mu^a \Gamma_a^{\mu\nu}(\theta)$. This expression is simplified by the identities (3.3) and (3.14), which yield

$$P_c(\theta) = t^a s_\nu \sigma_c^{\ dg} \nabla_d \theta_a^\nu - t_c s_\nu \sigma^{bdg} \nabla_b \theta_d^\nu + s_c t_\nu \sigma^{bdg} \nabla_b \theta_d^\nu. \tag{3.87}$$

Thus, we have the following main result.

Theorem 3.2. For the intrinsic Dirichlet boundary condition (3.77), a Hamiltonian conjugate to ξ^a on Σ is given by

$$H_{\Sigma}(\xi;\theta) = 8 \int_{\Sigma} \xi^{e} n_{\mu} (R_{e}^{\mu}(\theta) - \frac{1}{2} \theta_{e}^{\mu} R(\theta)) d\Sigma + 8 \int_{\partial \Sigma} \xi^{c} P_{c}(\theta) dS.$$
 (3.88)

On vacuum solutions θ_a^{μ} , the Hamiltonian reduces to the surface integral (3.86), (3.87).

Note, this Hamiltonian is unique up to adding an arbitrary covector function of the Dirichlet boundary data $h_{\mu}^{\ a}$ to $P_c(\theta)$.

D. Dirichlet Hamiltonian

On vacuum solutions of the Einstein equations, the Hamiltonian (3.88) with the Dirichlet boundary condition (3.77) holding on the timelike hypersurface \mathcal{B} bounding a local spacetime region \mathcal{V} takes a simple form if the frame θ_a^{μ} is adapted to the boundary 2-surfaces $\partial \Sigma_t$ and ξ^a . Let

$$\boldsymbol{\vartheta}_{a}^{0} = t_{a}, \boldsymbol{\vartheta}_{a}^{1} = s_{a}, \boldsymbol{\vartheta}_{[a}^{2} \boldsymbol{\vartheta}_{b]}^{3} = \epsilon_{ab}, \boldsymbol{\vartheta}_{a}^{2} = \epsilon_{a}^{b} \boldsymbol{\vartheta}_{b}^{3} \tag{3.89}$$

which defines a preferred orthonormal frame ϑ_a^{μ} . It follows that

$$t^{\nu} = t^{a} \vartheta_{a}^{\nu} = -\delta_{0}^{\nu}, \ s^{\nu} = s^{a} \vartheta_{a}^{\nu} = \delta_{1}^{\nu}. \tag{3.90}$$

This choice of frame is unique up to rotations of $\vartheta_a^2, \vartheta_a^3$.

Theorem 3.3. For the Dirichlet boundary condition (3.77), the Hamiltonian (3.88) conjugate to ξ^a on Σ , evaluated in the orthonormal frame (3.89) for vacuum solutions ϑ_a^{μ} , is given by the surface integral

$$H^{D}(\xi; \vartheta) = 8 \int_{\partial \Sigma} \xi^{c} P_{c}^{D}(\vartheta) dS$$
(3.91)

where

$$P_c^{\rm D}(\vartheta) = t^a \sigma_c^{\ dg} \nabla_d s_a - t_c \sigma^{bdg} \nabla_b s_d + s_c \sigma^{bdg} \nabla_b t_d. \tag{3.92}$$

We refer to $H^{\mathcal{D}}(\xi;\vartheta)$ as the *Dirichlet Hamiltonian* for the gravitational field in the local spacetime region \mathcal{V} , and $P_c^{\mathcal{D}}(\vartheta)$ as the *Dirichlet symplectic vector* associated to the boundary 2-surfaces $\partial \Sigma_t$. Note that, since ξ^a lies in \mathcal{B} , only the first two terms in $P_c^{\mathcal{D}}(\vartheta)$ contribute to $H^{\mathcal{D}}(\xi;\vartheta)$. The significance of the full expression for $P_c^{\mathcal{D}}(\vartheta)$ and its resulting geometrical properties are discussed in Ref. [8].

The general form of the Hamiltonian boundary term (3.86) and (3.87) differs from the special form (3.91) and (3.92) when evaluated in an orthonormal frame not adapted to $\partial \Sigma_t$ and ξ^a . In particular, we obtain the relation

$$P_c(\theta) = P_c^{D}(\theta) - \sigma_c^d t^{\nu} \partial_d s_{\nu} + t_c \sigma^{b\nu} \partial_b s_{\nu} - s_c \sigma^{b\nu} \partial_b t_{\nu}$$
(3.93)

and so the general form of the symplectic vector $P_c(\theta)$ differs from $P_c^{\rm D}(\vartheta)$ by various gradient terms. These terms can be understood by considering a change of orthonormal frame

$$\theta_a^\mu \to U^\mu_{\nu} \theta_a^\nu$$
 (3.94)

where $U^{\mu}_{\ \nu}$ is a SO(3,1) transformation acting in the frame bundle of the spacetime (M,g) at $\partial \Sigma_t$. Such transformations are defined by $U^{-1\mu}_{\ \nu} = U^{\alpha}_{\ \beta} \eta_{\alpha\nu} \eta^{\mu\beta}$ and $\det(U) = 1$, where $U^{-1\mu}_{\ \nu}$ is the inverse of $U^{\mu}_{\ \nu}$, given by $U^{-1\mu}_{\ \nu} U^{\nu}_{\ \alpha} = \delta^{\mu}_{\ \alpha} = U^{\mu}_{\ \nu} U^{-1\nu}_{\ \alpha}$.

The transformations (3.94) are a gauge symmetry of the tetrad formulation for General Relativity. Under the change of orthonormal frame, one has

$$\Gamma_{a\mu}{}^{\nu}(\theta) = \theta_{\mu}^{b\,g} \nabla_{a} \theta_{b}^{\nu} \to \Gamma_{a\mu}{}^{\nu}(U\theta) = U^{-1\alpha}{}_{\mu} \theta_{\alpha}^{b\,g} \nabla_{a} (U^{\nu}{}_{\beta} \theta_{b}^{\beta}) = U^{-1\alpha}{}_{\mu} U^{\nu}{}_{\beta} \Gamma_{a\alpha}{}^{\beta}(\theta) + U^{-1\alpha}{}_{\mu} \partial_{a} U^{\nu}{}_{\alpha},$$

$$(3.95)$$

and so, through substitution of the transformation (3.95) into the curvature (3.51),

$$R_{ab\mu}^{\nu}(\theta) \to R_{ab\mu}^{\nu}(U\theta) = U^{-1\alpha}_{\mu} U^{\nu}_{\beta} R_{ab\alpha}^{\beta}(\theta) \tag{3.96}$$

after cancellations of terms. Hence the Lagrangian (3.52) for the field variable θ_a^μ is gauge invariant. As a consequence, it is straightforward to see that the symplectic structure given by the symplectic potential (3.55) and current (3.66) must be gauge invariant. In particular, note that one has $\delta \Gamma_{a\mu}^{\nu}(U\theta) = U^{-1\alpha}_{\mu}U^{\nu}_{\beta}\delta\Gamma_{a\alpha}^{\beta}(\theta)$ where the gradient term from Eq. (3.95) drops out of the variation since it has no dependence on θ_a^μ . This explicitly establishes the gauge invariance of $\Theta_{abc}(\theta,\delta\theta)$ and hence of $\omega_{abc}(\theta,\delta_1\theta,\delta_2\theta)$.

However, the Noether charge (3.63) fails to be gauge invariant due to its explicit dependence on the frame connection. Consequently, it follows that the gradient terms in the symplectic vector (3.93) originate from a gauge transformation on the frame connection under (3.94) as given by a transformation relating the adapted orthonormal frame to a general orthonormal frame, $\theta_a^{\mu} = U^{\mu}_{0} t_a + U^{\mu}_{1} \sigma_a^{1} + U^{\mu}_{2} \sigma_a^{2} + U^{\mu}_{4} s_a$.

The gauge invariance of the symplectic structure arising from the tetrad formulation of the Lagrangian means that the symplectic potential (3.55) and current (3.66) are equivalent to manifestly gauge-invariant expressions derived using the metric formulation of General Relativity with g_{ab} as the field variable. It can be shown that one has

$$\Theta_{abc}(g, \delta g) = \Theta_{abc}(\theta, \delta \theta) + 6\partial_{[c}\psi_{ab]}(g, \delta g) \tag{3.97}$$

where $\psi_{ab}(g,\delta g)$ is a locally constructed 2-form, and so the symplectic potentials are equivalent to within an exact 3-form. This contributes a boundary term to the presymplectic form obtained from the metric Lagrangian $L_{abcd}(g) = \epsilon_{abcd}(g)R(g)$,

$$\Omega_{\Sigma}(g, \delta g, \mathcal{L}_{\xi}g) = \Omega_{\Sigma}(\theta, \delta \theta, \mathcal{L}_{\xi}\theta) + \int_{\partial \Sigma} \epsilon^{ab} (\delta \psi_{ab}(g, \mathcal{L}_{\xi}g) - \mathcal{L}_{\xi}\psi_{ab}(g, \delta g)) dS.$$
 (3.98)

Correspondingly, the Noether charge 2-form $Q_{ab}(\xi, g)$ arising in the metric formulation differs from $Q_{ab}(\xi, \theta)$ in the tetrad formulation by the term $2\psi_{ab}(g, \mathcal{L}_{\xi}g)$. Explicitly, using the metric Lagrangian, one finds that [11]

$$\frac{1}{4} \epsilon^{ab} Q_{ab}(\xi, g) = -4t_{[c} s_{d]}{}^{g} \nabla^{c} \xi^{d} = 4\xi^{d} t^{cg} \nabla_{c} s_{d} - 2(s^{c} \mathcal{L}_{\xi} t_{c} + t^{c} \mathcal{L}_{\xi} s_{c}). \tag{3.99}$$

Here the first term in Eq. (3.99) is simply the Noether charge (3.63) evaluated in the adapted orthonormal frame (3.89),

$$\epsilon^{ab}Q_{ab}(\xi,\vartheta) = 4\xi^c\Gamma_c^{\ \mu\nu}(\vartheta)\epsilon^{ab}\epsilon_{abmn}(g)\vartheta_\mu^m\vartheta_\nu^n = 16\xi^ct_\mu s_\nu\vartheta^{b\mu g}\nabla_c\vartheta_b^\nu = 16\xi^ct^{dg}\nabla_c s_d \qquad (3.100)$$

since $\mathcal{P}_{\mathcal{B}}({}^{g}\nabla_{[c}s_{d]}) = 0$ by hypersurface orthogonality of s_{d} . The second term in Eq. (3.99) simplifies through the hypersurface orthogonality relations (3.6) and (3.7), leading to

$$t^{c}\mathcal{L}_{\xi}s_{c} = t^{c}(2\xi^{bg}\nabla_{[b}s_{c]} + \partial_{c}(\xi^{b}s_{b})) = 0$$
(3.101)

and

$$s^{c}\mathcal{L}_{\xi}t_{c} = -\xi^{a}\frac{N}{\alpha}\partial_{a}\beta \tag{3.102}$$

where α, β, N are scalar functions defined by

$$s_a = \alpha \partial_a s, \quad t_a = -N(\partial_a t + \beta \partial_a s) \tag{3.103}$$

with

$$\mathcal{L}_{\xi}t = \xi^e \partial_e t = 1, \quad \mathcal{L}_{\xi}s = \xi^e \partial_e s = 0. \tag{3.104}$$

Hence we obtain the relation

$$\epsilon^{ab}Q_{ab}(\xi,g) = \epsilon^{ab}Q_{ab}(\xi,\vartheta) + 8\xi^a \frac{N}{\alpha} \partial_a \beta. \tag{3.105}$$

A similar relation can be shown to hold between the respective symplectic vectors arising in the tetrad and metric Hamiltonian formulations of General Relativity. In particular, by direct calculation with g_{ab} as the field variable, one finds that the full Dirichlet boundary condition (3.34) yields a Hamiltonian conjugate to ξ^a on Σ whose boundary term is given by

$$H^{\mathcal{D}}(\xi;g) = 8 \int_{\partial \Sigma} \xi^{c} P_{c}^{\mathcal{D}}(g) dS$$
(3.106)

where

$$P_c^{\rm D}(g) = P_c^{\rm D}(\vartheta) + \frac{N}{\alpha} \partial_c \beta. \tag{3.107}$$

This differs from the symplectic vector in the tetrad formulation by the same gradient term occurring in the Noether charges (3.105). The extrinsic part (3.38) of the Dirichlet boundary condition is necessary in obtaining this Hamiltonian, because of the boundary term in the presymplectic form (3.98). Interestingly, in the case when ξ^a is orthogonal to Σ_t , then $\beta = 0$, and one finds that the weaker, intrinsic Dirichlet boundary condition (3.37) is sufficient for existence of the metric Hamiltonian (3.106) and (3.107). Moreover, in this case the presymplectic form (3.98) and symplectic vector (3.107) are exactly the same as those obtained in the tetrad formulation using the adapted orthonormal frame (3.89).

An expression for the Dirichlet Hamiltonian boundary term (3.106) in terms of the standard ADM canonical variables associated to Σ , and its relation to quasilocal quantities of Brown and York [16,17], will be derived in Sec. III F.

E. Determination of allowed boundary conditions

A necessary and sufficient condition [10] on variations $\delta\theta_a^{\mu}$ for existence of a Hamiltonian (3.76) conjugate to ξ^a on Σ is given by the antisymmetrized variation of the equation (3.72) for the boundary term. This yields

$$\epsilon^{ab}\xi^{c}\omega_{abc}(\theta,\delta_{1}\theta,\delta_{2}\theta)|_{\partial\Sigma} = \sigma_{a}^{b}\partial_{b}\tilde{\beta}^{a}(\xi,\theta;\delta_{1}\theta,\delta_{2}\theta)|_{\partial\Sigma}$$
(3.108)

with

$$\tilde{\beta}^{a}(\xi,\theta;\delta_{1}\theta,\delta_{2}\theta) = \epsilon^{ab}\delta_{1}\alpha_{b}(\xi,\theta;\delta_{2}\theta) - \epsilon^{ab}\delta_{2}\alpha_{b}(\xi,\theta;\delta_{1}\theta). \tag{3.109}$$

To begin, we simplify the expression (3.66) for $\omega_{abc}(\theta, \delta_1 \theta, \delta_2 \theta)$. First, using Eq. (3.74) for $\Theta_{abc}(\theta, \delta\theta)$ and taking into account the orthogonality $\xi^a s_a = 0$, we have

$$\frac{1}{16} \epsilon^{ab} \xi^c \Theta_{abc}(\theta, \delta \theta) = \xi^c t_c h_\mu^{\ a} \delta(s_\nu h^{b\mu g} \nabla_a \theta_b^\nu) \tag{3.110}$$

through the frame decomposition (3.41) and the relation $\Gamma_a^{\ \mu\nu}(\theta)=\theta^{c\mu g}\nabla_a\theta^{\nu}_c=-\theta^{c\nu g}\nabla_a\theta^{\mu}_c$. Now we substitute the identity ${}^g\nabla_a\theta^{\nu}_b=h_a^{\ cg}\nabla_c\theta^{\nu}_b-s_as^{cg}\nabla_c\theta^{\nu}_b$ and then use the relations $h^{a\mu}\delta s_a=0$, $h^{a\mu}s_a=0$ to simplify the term

$$h_{\mu}^{\ a}\delta(s_{\nu}s_{a}h^{b\mu}s^{cg}\nabla_{c}\theta_{b}^{\nu}) = 0. \tag{3.111}$$

Thus, Eq. (3.110) becomes

$$\frac{1}{16} \epsilon^{ab} \xi^c \Theta_{abc}(\theta, \delta \theta) = \xi^c t_c h^{a\mu} \delta(s_{\nu} h_{\mu}^{\ b} h_a^{\ cg} \nabla_c \theta_b^{\nu}). \tag{3.112}$$

Finally, we substitute $\xi^c t_c = \frac{1}{2} \epsilon^{ab} \xi^c \epsilon_{abc}(h)$.

Hence, we obtain

$$\mathcal{P}_{\mathcal{B}}\Theta_{abc}(\theta,\delta\theta) = 8\epsilon_{abc}(h)h_{\mu}^{d}\delta K_{d}^{\mu} \tag{3.113}$$

where we define

$$K_a^{\ \mu} = s_{\nu} h^{b\mu} h_a^{\ cg} \nabla_c \theta_b^{\nu} = s_{\nu} h_a^{\ c} \Gamma_c^{\ \mu\nu}(\theta).$$
 (3.114)

Note that $s^a K_a^{\ \mu} = 0$ and $s_{\mu} K_a^{\ \mu} = 0$. From Eq. (3.113), by taking an antisymmetric variation and then using Eq. (3.46) for the variation of $\epsilon_{abc}(h)$, we have

$$\mathcal{P}_{\mathcal{B}}\omega_{abc}(\theta, \delta_{1}\theta, \delta_{2}\theta)$$

$$= 8\epsilon_{abc}(h) \left((\delta_{1}h_{\mu}^{\ d} - h_{\mu}^{\ d}h_{e}^{\ \nu}\delta_{1}h_{\nu}^{\ e})\delta_{2}K_{d}^{\ \mu} - (\delta_{2}h_{\mu}^{\ d} - h_{\mu}^{\ d}h_{e}^{\ \nu}\delta_{2}h_{\nu}^{\ e})\delta_{1}K_{d}^{\ \mu} \right). \tag{3.115}$$

Substitution of this expression into equation (3.108) yields the following result.

Theorem 3.4. A Hamiltonian conjugate to ξ^a on Σ exists for variations $\delta\theta^{\mu}_a$ with support on $\partial\Sigma$ if and only if

$$\left((\delta_{1}h_{\mu}^{\ d} - h_{\mu}^{\ d}h_{e}^{\ \nu}\delta_{1}h_{\nu}^{\ e})\delta_{2}K_{d}^{\ \mu} - (\delta_{2}h_{\mu}^{\ d} - h_{\mu}^{\ d}h_{e}^{\ \nu}\delta_{2}h_{\nu}^{\ e})\delta_{1}K_{d}^{\ \mu} \right) \Big|_{\partial\Sigma}
= \frac{1}{16N}\sigma_{a}^{\ b}\partial_{b}\tilde{\beta}^{a}(\xi,\theta;\delta_{1}\theta,\delta_{2}\theta)|_{\partial\Sigma}$$
(3.116)

for some $\tilde{\beta}^a(\xi,\theta;\delta_1\theta,\delta_2\theta)$ of the form (3.109). The Hamiltonian is given by

$$H_{\Sigma}(\xi;\theta) = 8 \int_{\Sigma} \xi^{e} n_{\mu} (R_{e}^{\ \mu}(\theta) - \frac{1}{2} \theta_{e}^{\mu} R(\theta)) d\Sigma + H_{B}(\xi;\theta)$$
 (3.117)

with boundary term

$$H_B(\xi,\theta) = \int_{\partial \Sigma} Q_{ab}(\xi,\theta) - \xi^c \tilde{B}_{abc}(\theta)$$
 (3.118)

where $\tilde{B}_{abc}(\theta)$ is determined from the equation

$$\xi^{c}(\mathcal{P}_{\mathcal{B}}\delta\tilde{B}_{abc}(\theta) - 8\epsilon_{abc}(h)h_{\mu}^{\ \ d}\delta K_{d}^{\ \mu}) = \mathcal{P}_{\mathcal{B}}\partial_{[a}\alpha_{b]}(\xi, \theta; \delta\theta). \tag{3.119}$$

Thus, equation (3.116) determines the allowed boundary conditions on variations $\delta\theta_a^{\mu}$ for existence of a Hamiltonian formulation (3.117) for the vacuum Einstein equations. To proceed, we now parallel the analysis of the similar boundary condition determining equation for the Maxwell equations in Sec. II C.

Two obvious solutions of the determining equation (3.116) with $\tilde{\beta}^a(\xi,\theta;\delta_1\theta,\delta_2\theta)=0$ are given by $\delta h_{\mu}^{\ a}|_{\partial\Sigma_t}=0, t\geq 0$, which is the Dirichlet boundary condition (3.77) already considered; and by

$$\delta K_a^{\mu}|_{\partial \Sigma_t} = 0, \quad t \ge 0 \tag{3.120}$$

which we call the *Neumann boundary condition*. For the boundary condition (3.120), it follows from Eqs. (3.76) and (3.119) that the corresponding Hamiltonian boundary term is given by

$$H^{N}(\xi;\theta) = 8 \int_{\partial \Sigma} \xi^{c} P_{c}^{N}(\theta) dS$$
(3.121)

where

$$P_c^{N}(\theta) = t_{\mu} s_{\nu} \Gamma_c^{\mu\nu}(\theta) = t^a s_{\nu}^{g} \nabla_c \theta_a^{\nu}$$

$$(3.122)$$

by a derivation similar to Eq. (3.87). In the orthonormal frame (3.89) adapted to the boundary 2-surfaces $\partial \Sigma_t$, we have

$$P_c^{N}(\vartheta) = t^{ag} \nabla_c s_a \tag{3.123}$$

We refer to this as the Neumann symplectic vector associated to the boundary 2-surfaces $\partial \Sigma_t$. Moreover, in this frame the Neumann boundary condition (3.120) becomes

$$\delta K_a^{\mu}|_{\partial \Sigma_t} = \delta(h^{b\mu}K_{ab})|_{\partial \Sigma_t} = 0, \quad t \ge 0$$
(3.124)

in terms of

$$K_{ab} = h_a^{\ c} h_b^{\ dg} \nabla_c s_d \tag{3.125}$$

which is the extrinsic curvature of the timelike boundary hypersurface \mathcal{B} in (M, g). Thus, geometrically, the Neumann boundary condition corresponds to fixing the frame components of the boundary hypersurface extrinsic curvature,

$$\delta(h^{b\mu}h_a{}^{cg}\nabla_c s_b) = 0 \quad \text{on } \mathcal{B}. \tag{3.126}$$

These components measure the rotation and boost of the hypersurface normal s_a with respect to the frame $h_a^{\ \mu}$ under displacement on \mathcal{B} .

We now investigate more general boundary conditions. Note that, on the left-side of the determining equation (3.116), $\epsilon^{ab}\xi^c\omega_{abc}(\theta,\delta_1\theta,\delta_2\theta)$ involves only the field variations $\mathcal{P}_{\mathcal{B}}\delta h_{\mu}^{\ a}$ and $\mathcal{P}_{\mathcal{B}}\delta K_a^{\ \mu} = \mathcal{P}_{\mathcal{B}}\delta(s_{\nu}h_a^{\ c}\Gamma_a^{\ \mu\nu}(\theta))$. We call $h_{\mu}^{\ a}$ and $K_a^{\ \mu}$ the symplectic boundary data at $\partial \Sigma_t$ and consider boundary conditions of the form

$$\delta \mathcal{F}_{a}^{\mu}(h_{c}^{\nu}, K_{c}^{\nu})|_{\partial \Sigma_{t}} = 0, t \geq 0$$
 (3.127)

where $\mathcal{F}_a^{\mu}(h_c^{\ \nu}, K_c^{\ \nu})$ is locally constructed as an algebraic expression in terms of the symplectic boundary data and fixed quantities (including the spacetime coordinates). We call (3.127) a mixed Dirichlet-Neumann boundary condition if $\mathcal{F}_a^{\mu}(h_c^{\ \nu}, K_c^{\ \nu})$ is a constant-coefficient linear combination of the parts $\mathcal{P}_{\partial\Sigma}h_a^{\ \mu}$, $\mathcal{P}_th_a^{\ \mu}$, $\mathcal{P}_{\partial\Sigma}K_a^{\ \mu}$, $\mathcal{P}_tK_a^{\ \mu}$ of the Dirichlet and Neumann boundary data in (3.77) and (3.120). Here the projections with respect to $\mathcal{P}_{\partial\Sigma}$ and \mathcal{P}_t remove all components proportional to s_a .

An analysis of the boundary condition determining equation (3.116), given later, leads to the following main results.

Theorem 3.5. The only allowed mixed Dirichlet-Neumann boundary conditions for existence of a Hamiltonian (3.76) conjugate to ξ^a on Σ are given by

$$\mathcal{P}_{\mathcal{B}}(a_0 \delta K_a^{\ \mu} + b_0 \delta h_a^{\ \mu})|_{\partial \Sigma_t} = 0, \quad t \ge 0,$$
 (3.128)

or equivalently

$$\mathcal{F}_{a}^{\mu}(h_{c}^{\nu}, K_{c}^{\nu}) = a_{0}K_{a}^{\mu} + b_{0}h_{a}^{\mu} \tag{3.129}$$

for constants a_0, b_0 (and $\beta^a = 0$ in Eq. (3.116)). In the cases $a_0 = 0$ or $b_0 = 0$, respectively Dirichlet or Neumann boundary conditions, the corresponding Hamiltonian boundary terms are given by Eqs. (3.91) and (3.87), and Eqs. (3.121) and (3.122). In the case $a_0 \neq 0, b_0 \neq 0$, the corresponding Hamiltonian boundary term is given by

$$H^{\mathrm{DN}}(\xi;\theta) = 8 \int_{\partial \Sigma} \xi^{c} P_{c}(\theta) dS \tag{3.130}$$

where, now,

$$P_c(\theta) = P_c^N(\theta) + 6\frac{b_0}{a_0}t_c. {(3.131)}$$

(Note, the boundary terms here are unique up to adding an arbitrary covector function of the boundary data (3.129) to $P_c(\theta)$.)

A similar covariant derivation of the pure Dirichlet and Neumann boundary terms is presented in Ref. [18,19] from a different perspective. In Theorem 3.5, note that Eq. (3.128) represents a one-parameter a_0/b_0 family of boundary conditions. In particular, in contrast to the two-parameter family of analogous mixed Dirichlet-Neumann boundary conditions (2.52) allowed for the Maxwell equations, here decompositions of the symplectic boundary data with respect to $\mathcal{P}_{\partial\Sigma}$ and \mathcal{P}_{ξ} do not yield boundary conditions satisfying the determining equation (3.116).

The form of the mixed Dirichlet-Neumann boundary condition (3.128) suggests we also consider boundary conditions specified by a trace part and trace-free part with respect to the boundary hypersurface frame $h_a^{\ \mu}$:

$$\delta \hat{\mathcal{F}}(h_c^{\nu}, K_c^{\nu})|_{\partial \Sigma_t} = 0, \quad \delta \hat{\mathcal{F}}_a^{\mu}(h_c^{\nu}, K_c^{\nu})|_{\partial \Sigma_t} = 0, \quad t \ge 0$$
 (3.132)

with $h_{\mu}^{\ a}\hat{\mathcal{F}}_{a}^{\mu}(h_{c}^{\ \nu},K_{c}^{\ \nu})=0$. Taking the trace of the symplectic boundary data variations yields

$$h_{\mu}{}^{a}\delta K_{a}{}^{\mu} = \delta K + h_{\mu}{}^{b}h_{\nu}{}^{a}K_{a}{}^{\mu}\delta h_{b}{}^{\nu}$$
(3.133)

and

$$h_{\mu}^{\ a}\delta h_{a}^{\ \mu} = \delta \ln|h| \tag{3.134}$$

where $K=h_{\mu}{}^aK_a{}^{\mu}$ is the trace of $K_a{}^{\mu}$ and $h=\det(h_a{}^{\mu})$ is the determinant of the frame components $h_a{}^{\mu}$ in local coordinates.

Theorem 3.6. Allowed boundary conditions (3.132) for the existence of a Hamiltonian (3.76) conjugate to ξ^a on Σ are given by

$$\mathcal{P}_{\mathcal{B}}\delta(K_a^{\ \mu} - \frac{1}{3}h_a^{\ \mu}K)|_{\partial\Sigma_t} = 0, \quad t \ge 0, \tag{3.135}$$

$$(a_0 \delta K + b_0 \delta \ln|h|)|_{\partial \Sigma_t} = 0, \quad t \ge 0,$$
 (3.136)

or equivalently

$$\hat{\mathcal{F}}(h,K) = a_0 K + b_0 \ln|h|, \quad \hat{\mathcal{F}}_a^{\mu}(h_c^{\nu}, K_c^{\nu}) = \mathcal{P}_{\mathcal{B}}(K_a^{\mu} - \frac{1}{3}h_a^{\mu}K)$$
(3.137)

for constants a_0, b_0 (and $\beta^a = 0$ in Eq. (3.116)). The corresponding Hamiltonian boundary term is given by

$$H_B(\xi,\theta) = 8 \int_{\partial \Sigma} \xi^c (\frac{1}{3} P_c^D(\theta) + \frac{2}{3} P_c^N(\theta) + 4 \frac{b_0}{a_0} t_c) dS$$
 (3.138)

(which is unique up to adding a term depending on an arbitrary covector function of the boundary data (3.137)).

Finally, we remark that the mixed boundary conditions in Theorems 3.5 and 3.6 admit the following two generalizations.

First,

$$\hat{\mathcal{F}}_{a}^{\mu}(h_{c}^{\nu}, K_{c}^{\nu}) = a(x, K, \ln|h|) \mathcal{P}_{\mathcal{B}}(K_{a}^{\mu} - \frac{1}{3}h_{a}^{\mu}K), \tag{3.139}$$

$$\hat{\mathcal{F}}(h,K) = b(x,K,\ln|h|), \quad \partial_K b \neq 0 \tag{3.140}$$

for arbitrary functions $a(x, K, \ln |h|), b(x, K, \ln |h|)$.

Second,

$$\mathcal{F}_{a}^{\mu}(h_{c}^{\nu}, K_{c}^{\nu}) = a(x, K, \ln|h|) \mathcal{P}_{\mathcal{B}}(K_{a}^{\mu} + b(x, K, \ln|h|) h_{a}^{\mu}), \quad b \neq -\frac{1}{3}K$$
 (3.141)

for an arbitrary function $b(x, K, \ln |h|)$, with the function $a(x, K, \ln |h|)$ now satisfying the linear partial differential equation

$$(\partial_K \hat{b}) \partial_{\ln|h|} a + (\hat{b} + \partial_{\ln|h|} \hat{b}) \partial_K a = \frac{2}{9} (-1 + 3\partial_K \hat{b}) a, \quad \hat{b} = b + \frac{1}{3} K \tag{3.142}$$

obtained from the determining equation (3.116). The general form of a is given by solving the characteristic ordinary differential equations

$$\frac{d\ln|h|}{\partial_{_{K}}\hat{b}} = \frac{dK}{\hat{b} + \partial_{\ln|h|}\hat{b}} = \frac{da}{\frac{2}{9}(-1 + 3\partial_{_{K}}\hat{b})a}$$
(3.143)

in terms of the variables $\ln |h|, K, a$. For instance, if b is taken to be linear homogeneous in K, then one has $b = \lambda K$, $a = f(x, \lambda K \ln |h|) |h|^{\frac{2}{3} \frac{\lambda}{3\lambda - 1}}$, where $\lambda = \text{const}$ and f is an arbitrary function.

Proofs of Theorems:

Since any boundary condition locally constructed from the symplectic boundary data is linear homogeneous in $\mathcal{P}_{\mathcal{B}}\delta h_a^{\ \mu}$ and $\mathcal{P}_{\mathcal{B}}\delta K_a^{\ \mu}$, we begin by finding all such solutions of the determining equation (3.116).

First we show that $\tilde{\beta}^a = 0$. The right-side of Eq. (3.116) necessarily involves terms with at least one derivative on $\delta\theta_a^{\mu}$, while only first-order derivatives of $\delta\theta_a^{\mu}$ appear on the left-side of Eq. (3.116) through

$$\mathcal{P}_{\mathcal{B}}\delta K_{a}^{\ \mu} = s_{\nu}h_{a}^{\ c}\delta\Gamma_{c}^{\ \mu\nu}(\theta) \tag{3.144}$$

due to Eqs. (3.114) and (3.47). Thus, for a balance in numbers of derivatives, we must have

$$\alpha_a = \alpha_{a\mu}^{\ b}(\theta)\delta\theta_b^{\mu} \tag{3.145}$$

for some $\alpha_{a\mu}^{\ b}(\theta)$ locally constructed out of θ_a^{μ} and fixed quantities. This yields, for the antisymmetrized variation of α_a ,

$$\beta_a = \alpha_{au\nu}^{\ bc}(\theta)\delta_1\theta_b^{\mu}\delta_2\theta_c^{\nu} \tag{3.146}$$

where $\alpha_{a\mu\nu}^{\ bc}(\theta)=-\alpha_{a\nu\mu}^{\ cb}(\theta)$ is the curl of $\alpha_{a\mu}^{\ b}(\theta)$ with respect to θ_c^{ν} . Then, using Eqs. (3.109) and (3.50), we collect all the terms on the left-side of Eq. (3.116) linearly independent of $\delta h_a^{\ \mu}$, $\delta K_a^{\ \mu}$. Through Eqs. (3.144) and (3.49), the coefficients of these terms yield

$$s_c \tilde{\alpha}^{(be)c}_{\mu\nu}(\theta) = 0, \quad s_b \tilde{\alpha}^{[be]c}_{\mu\nu}(\theta) = 0, \quad s_c \tilde{\alpha}^{[be]c}_{\mu\nu}(\theta) = 0$$
 (3.147)

where

$$\tilde{\alpha}^{ebc}_{\ \mu\nu}(\theta) = \epsilon^{ae} \alpha^{bc}_{a\mu\nu}(\theta) = -\tilde{\alpha}^{ecb}_{\ \nu\mu}(\theta). \tag{3.148}$$

These algebraic equations are straightforward to solve, leading to

$$\alpha_{\mu\nu}^{abc}(\theta) = t^{[b}\alpha_{1\mu\nu}^{c]a}(\theta) + \alpha_{2\mu\nu}^{abc}(\theta) + t^{b}t^{c}\alpha_{3\mu\nu}^{a}(\theta) + t^{(b}\alpha_{4\mu\nu}^{c)a}(\theta)$$
(3.149)

for some

$$\alpha_{1\mu\nu}^{\ ca} = \sigma_b^{\ c} \sigma_d^{\ a} \alpha_{1(\mu\nu)}^{\ bd}, \ \alpha_{2\mu\nu}^{\ abc} = -\sigma_e^{\ a} \sigma_d^{\ b} \sigma_f^{\ c} \alpha_{2\nu\mu}^{\ edf}, \ \alpha_{3\mu\nu}^{\ a} = \sigma_e^{\ a} \alpha_{3[\mu\nu]}^{\ e}, \ \alpha_{4\mu\nu}^{\ ca} = \sigma_b^{\ c} \sigma_d^{\ a} \alpha_{4[\mu\nu]}^{\ bd}.$$

$$(3.150)$$

Then, returning to Eq. (3.145), we note that $\alpha_{a\mu}^{\ b}(\theta) = \theta_a^{\alpha} \theta_{\beta}^{\ b} \alpha_{\mu\alpha}^{\beta}$ for some $\alpha_{\mu\alpha}^{\beta}$ that is locally constructed only from fixed quantities since it is a scalar expression. Thus we immediately obtain

$$\alpha^{abc}_{\mu\nu}(\theta) = \theta^b_\beta \theta^c_\gamma \theta^{a\alpha} (\alpha^\beta_{\nu\mu} \delta^\gamma_\alpha - \alpha^\gamma_{\mu\nu} \delta^\beta_\alpha - \alpha^\gamma_{\alpha\mu} \delta^\beta_\nu + \alpha^\beta_{\alpha\mu} \delta^\gamma_\nu). \tag{3.151}$$

By equating expressions (3.149) and (3.151), we find that after some algebraic analysis

$$\alpha_{\nu\mu}^{\gamma} = \delta_{\nu}^{\gamma} \alpha_{0\mu} \tag{3.152}$$

for some $\alpha_{0\mu}$. Now, substitution of expression (3.152) back into Eqs. (3.149) and (3.151) easily leads to the result

$$\alpha_{1\mu\nu}^{ca} = \alpha_{2\mu\nu}^{abc} = \alpha_{3\mu\nu}^{a} = \alpha_{4\mu\nu}^{ca} = 0. \tag{3.153}$$

Hence, from Eq. (3.149), we have $\alpha_{a\mu\nu}^{\ bc}(\theta)=0$ and so $\beta_a=0$. This establishes that $\tilde{\beta}^a=0$. Consequently, the determining equation (3.116) reduces to

$$(\delta_1 h_{\mu}^{\ d} - h_{\mu}^{\ d} h_e^{\ \nu} \delta_1 h_{\nu}^{\ e}) \delta_2 K_d^{\ \mu} - (\delta_2 h_{\mu}^{\ d} - h_{\mu}^{\ d} h_e^{\ \nu} \delta_2 h_{\nu}^{\ e}) \delta_1 K_d^{\ \mu} = 0, \tag{3.154}$$

which is equivalent to

$$h_{[\nu}^{\ d}h_{\mu]}^{\ e}(\delta_1 h_e^{\ \nu} \delta_2 K_d^{\ \mu} - \delta_2 h_e^{\ \nu} \delta_1 K_d^{\ \mu}) = 0. \tag{3.155}$$

Then the algebraic solution of Eq. (3.155) in terms of $\mathcal{P}_{\mathcal{B}}\delta h_e^{\ \nu}$ and $\mathcal{P}_{\mathcal{B}}\delta K_d^{\ \mu}$ has the form

$$\Pi_{1a\nu}^{\mu b} \mathcal{P}_{\mathcal{B}} \delta h_b^{\nu} + \Pi_{2a\nu}^{\mu b} \mathcal{P}_{\mathcal{B}} \delta K_b^{\nu} = 0 \tag{3.156}$$

for some coefficient tensors $\Pi_{a\nu}^{\mu b}$ such that

$$\Pi^{\mu b}_{a\nu} h_{[\alpha}{}^a h_{\mu]}{}^c = \Pi^{\mu c}_{a\alpha} h_{[\nu}{}^a h_{\mu]}{}^b. \tag{3.157}$$

It is straightforward to show that Eq. (3.157) holds iff

$$\Pi_{a\nu}^{\mu b} = \hat{\Pi}_{a\nu}^{\mu b} - h_a^{\ \mu} \hat{\Pi}_{\nu}^{\ b} + h_{\nu}^{\ b} \hat{\Pi}_{a}^{\ \mu} \tag{3.158}$$

where $\hat{\Pi}_{a\nu}^{\ \mu b}h_{\alpha}^{\ a}h_{\mu}^{\ c}=\hat{\Pi}_{a\alpha}^{\ \mu c}h_{\nu}^{\ a}h_{\mu}^{\ b}$ is the symmetric part of $\Pi_{a\nu}^{\ \mu b}$ in the index pairs (a,μ) and (b,ν) , and where $\hat{\Pi}_{\nu}^{\ b}=h_{\mu}^{\ a}\hat{\Pi}_{a\nu}^{\ \mu b}, \hat{\Pi}_{a}^{\ \mu}=h_{b}^{\ \nu}\hat{\Pi}_{a\nu}^{\ \mu b}$ is the trace part of $\Pi_{a\nu}^{\ \mu b}$ in the frame $h_{a}^{\ \mu}$. Thus, we have established the following result.

Lemma 3.7. All solutions of the determining equation (3.116) for allowed boundary conditions that are linear homogeneous in $\mathcal{P}_{\mathcal{B}}\delta h_a^{\ \mu}$ and $\mathcal{P}_{\mathcal{B}}\delta K_a^{\ \mu}$ have the form (3.156) where the coefficient tensors are given by Eq. (3.158).

Now, for mixed Dirichlet-Neumann boundary conditions, we take

$$\Pi_{1a\nu}^{\mu b} = a_1(\mathcal{P}_{\partial\Sigma})_a^{\ b} \sigma_{\nu}^{\ \mu} + a_0(\mathcal{P}_t)_a^{\ b} t_{\nu} t^{\mu}$$
(3.159)

$$\Pi_{2a\nu}^{\mu b} = b_1(\mathcal{P}_{\partial\Sigma})_a^{\ b} \sigma_{\nu}^{\ \mu} + b_0(\mathcal{P}_t)_a^{\ b} t_{\nu} t^{\mu}$$
(3.160)

where a_0, a_1, b_0, b_1 are constants. Then the requirement (3.158) leads directly to

$$a_0 = a_1, \ b_0 = b_1.$$
 (3.161)

Substitution of Eqs. (3.159) to (3.161) into Eq. (3.156) yields the mixed Dirichlet-Neumann boundary conditions (3.128).

Finally, the other boundary conditions (3.135) and (3.136) arise from

$$\Pi_{1a\nu}^{\mu b} = \frac{1}{2} \frac{b_0}{a_0} h_a^{\mu} h_{\nu}^{\ b} - \frac{1}{3} K h_d^{\ e} h_{\nu}^{\ \mu}, \tag{3.162}$$

$$\Pi_{2a\nu}^{\ \mu b} = h_a^{\ b} h_{\nu}^{\ \mu}, \tag{3.163}$$

which are easily verified to satisfy the requirement (3.158).

This completes the proofs of Theorems 3.5 and 3.6. \square

As a concluding remark, we note that Lemma 3.7 yields the following necessary and sufficient determining equations for finding all boundary conditions (3.127).

Lemma 3.8. All allowed boundary conditions of the form $\mathcal{F}_a^{\mu}(h_c^{\ \nu}, K_c^{\ \nu})|_{\partial \Sigma} = 0$ for existence of a Hamiltonian conjugate to ξ^a on Σ are given by the solutions of the equations

$$\frac{\partial \mathcal{F}_a^{\mu}}{\partial h_{\nu}^{\nu}} h_{[\alpha}^{\ a} h_{\mu]}^{\ c} = \frac{\partial \mathcal{F}_a^{\mu}}{\partial h_{c}^{\ \alpha}} h_{[\nu}^{\ a} h_{\mu]}^{\ b}, \tag{3.164}$$

$$\frac{\partial \mathcal{F}_{a}^{\mu}}{\partial K_{b}^{\nu}} h_{[\alpha}{}^{a} h_{\mu]}{}^{c} = \frac{\partial \mathcal{F}_{a}^{\mu}}{\partial K_{c}^{\alpha}} h_{[\nu}{}^{a} h_{\mu]}{}^{b}. \tag{3.165}$$

We will leave a general analysis of the boundary condition determining equations (3.164) and (3.165) for elsewhere.

F. Relation between covariant and canonical Hamiltonians and boundary terms

To conclude this section, we first give a brief discussion of the Hamiltonian field equations for General Relativity using the covariant symplectic structure and Noether charge Hamiltonian in Sec. III C. Then we discuss the boundary terms in the Dirichlet and Neumann Hamiltonians expressed in standard ADM canonical variables.

For a Hamiltonian (3.76) conjugate to ξ^a on Σ , the associated field equations are obtained through the presymplectic form (3.69) by the variational principle

$$\Omega_{\Sigma}(\theta, \delta\theta, \mathcal{L}_{\xi}\theta) - H_{\Sigma}'(\xi; \theta, \delta\theta) = \int_{\Sigma} 8\xi^{d} n_{d} (R_{\mu}^{\ e}(\theta) - \frac{1}{2}\theta_{\mu}^{e}) \delta\theta_{e}^{\mu} \ d\Sigma = 0$$
 (3.166)

for arbitrary variations $\delta\theta_e^{\mu}|_{\Sigma}$. These field equations split into evolution equations and constraint equations with respect to Σ corresponding to a decomposition of θ_a^{μ} into dynamical and non-dynamical components determined by [4] the degeneracy of

$$\Omega_{\Sigma}(\theta, \delta_1 \theta, \delta_2 \theta) = \int_{\Sigma} \omega_{abc}(\theta, \delta_1 \theta, \delta_2 \theta) = \int_{\Sigma} \frac{1}{6} \epsilon^{abcd} n_d \omega_{abc}(\theta, \delta_1 \theta, \delta_2 \theta) d\Sigma. \tag{3.167}$$

For this purpose, it is convenient to partially fix the SO(3,1) local gauge freedom in θ_e^{μ} analogously to conditions (3.15) to (3.17) by choosing the frame components $n^{\mu} = n^a \theta_a^{\mu}$ to be fixed constants on M. Then, through a simplification of the symplectic current here similar to Eq. (3.115), we obtain

$$\frac{1}{48}\epsilon^{abcd}n_{d}\omega_{abc}(\theta,\delta_{1}\theta,\delta_{2}\theta) = -(\delta_{1}q_{\mu}^{d} - q_{\mu}^{d}q_{e}^{\nu}\delta_{1}q_{\nu}^{e})\delta_{2}p_{d}^{\mu} + (\delta_{2}q_{\mu}^{d} - q_{\mu}^{d}q_{e}^{\nu}\delta_{2}q_{\nu}^{e})\delta_{1}p_{d}^{\mu} \ (3.168)$$

where we define

$$q_a^{\ \mu} = \theta_a^{\mu} + n_a n^{\mu}, \quad p_a^{\ \mu} = n_{\nu} q^{b\mu} q_a^{\ cg} \nabla_c \theta_b^{\nu} = n_{\nu} q_a^{\ c} \Gamma_c^{\ \mu\nu}(\theta)$$
 (3.169)

with $q_{ab}=g_{ab}+n_an_b$, which are counterparts of $h_a^{\ \mu}, K_a^{\ \mu}$ associated to the spacelike hypersurface Σ . (Geometrically, $q_a^{\ \mu}$ is a frame for the hypersurface metric $q_{ab}=q_a^{\ \mu}q_b^{\ \nu}\eta_{\mu\nu}$, while $p_a^{\ \mu}$ represents the frame components of the hypersurface extrinsic curvature $\mathcal{K}_{ab}=q_a^{\ \mu}p_b^{\ \nu}\eta_{\mu\nu}=q_a^{\ c}q_b^{\ \nu}\nabla_c n_b$.) Hence, the degeneracy directions of the presymplectic form (3.167) are given by variations $\delta\theta_a^{\mu}$ satisfying

$$\delta(q_a^{\ \mu}/|q|) = \delta p_a^{\ \mu} = 0. \tag{3.170}$$

where $|q| = det(q_a^{\ \mu})$ and $\delta \ln |q| = q_{\nu}^{\ b} \delta q_b^{\ \nu}$. This immediately leads to the following result, analogous to the discussion in Sec. II A for the Maxwell equations.

Proposition 3.9. For a Hamiltonian $H_{\Sigma}(\xi;\theta)$ conjugate to ξ^a on Σ , let $\theta_{\ker \omega}$ denote the field components of θ^{μ}_a and $\Gamma_a^{\ \mu\nu}(\theta)$ invariant under the symplectic degeneracy directions (3.170), and let θ_{ω} denote the remaining field components modulo $\theta_{\ker \omega}$. Then there is corresponding decomposition of the Hamiltonian field equations given by $H'_{\Sigma}(\xi;\theta,\delta\theta_{\ker \omega})=0$ and $H'_{\Sigma}(\xi;\theta,\delta\theta_{\omega})=\Omega_{\Sigma}(\theta,\delta\theta_{\omega},\mathcal{L}_{\xi}\theta)$, which respectively yield

$$n^{a}R_{a}^{\ \mu}(\theta) - \frac{1}{2}n^{\mu}R(\theta) = 0, \tag{3.171}$$

$$q_a^{\ b} R_b^{\ \mu}(\theta) = 0. \tag{3.172}$$

These field equations arise equivalently by variation of $\mathcal{P}_n\theta_a^{\mu} = -n_a n^{\mu}$ and $\mathcal{P}_{\Sigma}\theta_a^{\mu} = q_a^{\mu}$ in the Lagrangian (3.52).

Equations (3.171) and (3.172) are the frame components of the standard 3+1 split of the vacuum Einstein equations [12] into constraint equations and time-evolution equations for the hypersurface metric q_{ab} . Thus, the Hamiltonian field equations given by the variational principle (3.166) constitute a covariant formulation of the standard ADM Hamiltonian equations for General Relativity.

With respect to the spacelike hypersurface Σ , one has a decomposition of ξ^a into normal and tangential parts

$$\xi^a = \mathcal{N}n^a + \mathcal{N}^a \tag{3.173}$$

where $\mathcal{N}^a = \mathcal{P}_{\Sigma}(\xi^a)$ and $\mathcal{N} = -\xi^a n_a$ define the lapse and shift of the time flow vector field ξ^a . By use of the Gauss-Codacci equations, we straightforwardly see that the volume part of a Hamiltonian (3.76) conjugate to ξ^a on Σ is given by the "pure constraint form" [11]

$$H(\xi;\theta) = 4 \int_{\Sigma} \mathcal{N}(\mathcal{R} + \mathcal{K}^2 - \mathcal{K}_{ab}\mathcal{K}^{ab}) + 2\mathcal{N}^c(\mathcal{D}^b\mathcal{K}_{bc} - \mathcal{D}_c\mathcal{K}) \ d\Sigma$$
 (3.174)

where \mathcal{R}_{ab} and \mathcal{K}_{ab} are the Ricci curvature and extrinsic curvature of the metric $\mathcal{P}_{\Sigma}g_{ab}=q_{ab}$, $\mathcal{R}=\mathcal{R}_a^{\ a}$ and $\mathcal{K}=\mathcal{K}_a^{\ a}$ are the corresponding scalar curvatures, and \mathcal{D}_a is the derivative operator associated with q_{ab} . (An analogous result holds more generally for any diffeomorphism covariant Lagrangian field theory [4].) This demonstrates, explicitly, that our covariant analysis of allowed boundary conditions and corresponding boundary terms for General Relativity in Secs. III B and III E is equivalent to a canonical analysis of the ADM Hamiltonian.

Now, consider Dirichlet or Neumann boundary conditions imposed at the 2-surfaces $\partial \Sigma_t$, for $t \geq 0$. On solutions of the Hamiltonian field equations, the total Hamiltonian $H_{\Sigma}(\xi;\theta)$ reduces, respectively, to the Dirichlet and Neumann boundary terms (3.91) and (3.121). Let u^a denote the outward unit normal to $\partial \Sigma_t$ in Σ_t . Let $\tilde{\vartheta}_a^{\mu}$ be an orthonormal frame adapted to Σ_t given by

$$\tilde{\vartheta}_a^0 = n_a, \tilde{\vartheta}_a^1 = u_a, \tilde{\vartheta}_{[a}^2 \tilde{\vartheta}_{b]}^3 = \epsilon_{ab}, \tilde{\vartheta}_a^2 = \epsilon_a^{\ b} \tilde{\vartheta}_b^3$$

$$(3.175)$$

which is related to the frame ϑ_a^{μ} adapted to \mathcal{B} by a boost in the normal space $T^{\perp}(\partial \Sigma_t)$ to the boundary 2-surface $\partial \Sigma_t$,

$$t^{a} = n^{a} \cosh \chi + u^{a} \sinh \chi, \quad s^{a} = u^{a} \cosh \chi + n^{a} \sinh \chi. \tag{3.176}$$

Through the corresponding boost relation (3.95) applied to the symplectic vectors (3.92) and (3.123), the Hamiltonian boundary terms take the respective form

$$\boldsymbol{\xi}^{c} \boldsymbol{P}_{c}^{\mathrm{D}}(\tilde{\boldsymbol{\vartheta}}) = \boldsymbol{\xi}^{c} (\boldsymbol{n}^{a} \boldsymbol{\sigma}_{c}^{\ dg} \boldsymbol{\nabla}_{d} \boldsymbol{u}_{a} - \boldsymbol{n}_{c} \boldsymbol{\sigma}^{bdg} \boldsymbol{\nabla}_{b} \boldsymbol{u}_{d} + \boldsymbol{u}_{c} \boldsymbol{\sigma}^{bdg} \boldsymbol{\nabla}_{b} \boldsymbol{n}_{d} - \boldsymbol{\sigma}_{c}^{\ dg} \boldsymbol{\nabla}_{d} \boldsymbol{\chi}), \tag{3.177}$$

$$\xi^{c} P_{c}^{N}(\tilde{\vartheta}) = \xi^{c} (n^{ag} \nabla_{c} u_{a} - {}^{g} \nabla_{c} \chi). \tag{3.178}$$

These expressions can be simplified in terms of the hypersurface metric q_{ab} , extrinsic curvature \mathcal{K}_{ab} , and acceleration $a_b = n^{eg} \nabla_e n_b$. We find that

$$\xi^{c} P_{c}^{D}(\tilde{\vartheta}) = \mathcal{N}\kappa - \mathcal{N}^{a} u^{b} \mathcal{K}_{ab} - \mathcal{N}_{\parallel}^{a} \partial_{a} \chi, \tag{3.179}$$

$$\boldsymbol{\xi}^{c}\boldsymbol{P}_{c}^{\mathrm{N}}(\tilde{\boldsymbol{\vartheta}}) = -\mathcal{N}\boldsymbol{u}^{b}\boldsymbol{a}_{b} - \mathcal{N}^{a}\boldsymbol{u}^{b}\boldsymbol{\mathcal{K}}_{ab} - \mathcal{N}\boldsymbol{\partial}_{t}\boldsymbol{\chi} - \boldsymbol{\mathcal{N}}_{\perp}\boldsymbol{u}^{a}\boldsymbol{\partial}_{a}\boldsymbol{\chi} - \boldsymbol{\mathcal{N}}_{\parallel}^{a}\boldsymbol{\partial}_{a}\boldsymbol{\chi}, \tag{3.180}$$

where $\mathcal{N}^a_{\parallel} = \mathcal{P}_{\partial\Sigma}(\mathcal{N}^a)$, $\mathcal{N}_{\perp} = u_a \mathcal{N}^a$ are the tangential and normal parts of the shift with respect to $\partial\Sigma_t$, and $\kappa = \sigma^{abg}\nabla_a u_b$ is the mean extrinsic curvature of $\partial\Sigma_t$ in Σ_t .

We note that this form of the Dirichlet and Neumann boundary terms (3.179) and (3.180) agrees with the canonical analysis of boundary terms for the ADM Hamiltonian carried out in Refs. [16,17]. Moreover, in the case when Σ_t is orthogonal to \mathcal{B} , i.e. $\chi=0$, the surface integral $\int_{\partial\Sigma} \xi^c P_c^{\mathrm{D}}(\tilde{\vartheta}) dS$ for suitable choice of ξ^c reproduces Brown and York's expressions for quasilocal energy, normal momentum, and tangential momentum quantities (respectively, $\mathcal{N}=1, \mathcal{N}^a=0$; $\mathcal{N}=0, \mathcal{N}^a_{\parallel}=0, \mathcal{N}_{\perp}=1$; $\mathcal{N}=\mathcal{N}_{\perp}=0, \mathcal{N}^a_{\parallel}\neq0$). Further discussion of quasilocal quantities associated to the Dirichlet and Neumann symplectic vectors (3.92) and (3.123) will be left for elsewhere.

IV. CONCLUDING REMARKS

In this paper we have given a mathematical investigation of boundary conditions on the gravitational field required for the existence of a well-defined covariant Hamiltonian variational principle for General Relativity when spatial boundaries are considered, with a fixed time-flow vector field. In particular, a main result is that we obtain a covariant derivation of Dirichlet, Neumann, and mixed type boundary conditions for the gravitational field in any fixed spatially bounded region of spacetime. We show that the resulting Dirichlet and Neumann Hamiltonians lead to covariant Hamiltonian field equations which are equivalent to the standard 3+1 split of the Einstein equations into constraint equations and time-evolution

equations. In addition, we obtain a uniqueness result for the allowed boundary conditions based on the covariant symplectic structure associated to the Einstein equations.

However, we do not address the purely analytical issue of whether the boundary-initial value problem for the Einstein equations is well-posed with these boundary conditions (i.e. do there exist solutions of the Einstein equations satisfying the boundary conditions, initial conditions, and constraints). For work in that direction, see e.g. Ref. [20].

A further interesting generalization of our results would be to treat a spacetime region whose spatial boundary is dynamical e.g. a black-hole horizon or Cauchy boundary. We note that boundary conditions for this situation may be investigated by allowing the time-flow vector field to depend on the spacetime metric instead of being a fixed quantity. This analysis will be pursued elsewhere.

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APPENDIX: NOETHER CHARGE METHOD

First of all, consider in n spacetime dimensions a general Lagrangian field theory for a set of fields denoted collectively by ϕ . It will be assumed that these fields are defined as sections of a vector bundle E over the spacetime manifold M, using local coordinates on M and E. The theory will be assumed to be described by a Lagrangian n-form $L(\phi)$ that is locally constructed out of the fields ϕ and their partial derivatives $\partial^k \phi$ to some finite order k (and fixed background structure, if any, on M and E).

The Lagrangian $L(\phi)$ provides a variational principle

$$S(\phi) = \int_{M} L(\phi) \tag{A1}$$

which yields the field equations $\mathcal{E}(\phi) = 0$ obtained as the stationary points of $S(\phi)$,

$$\delta S(\phi) = \int_{M} \delta L(\phi) = \int_{M} \mathcal{E}(\phi) \delta \phi = 0 \tag{A2}$$

under variations $\delta \phi$ of ϕ with compact support on M. For arbitrary variations $\delta \phi$, which are not restricted to have compact support, one then has a variational identity

$$L'(\phi, \delta\phi) \equiv \delta L(\phi) = \mathcal{E}(\phi)\delta\phi + d\Theta(\phi, \delta\phi) \tag{A3}$$

where $\Theta(\phi, \delta\phi)$ is an (n-1)-form, called the *symplectic potential*, derived through formal integration by parts. This yields a well-defined locally constructed formula for $\mathcal{E}(\phi)$ and $\Theta(\phi, \delta\phi)$ in terms of ϕ , $\delta\phi$, and their partial derivatives to a finite order. The symplectic potential is used to define the *presymplectic form* on a fixed hypersurface Σ ,

$$\Omega_{\Sigma}(\phi, \delta_1 \phi, \delta_2 \phi) \equiv \int_{\Sigma} \omega(\phi, \delta_1 \phi, \delta_2 \phi) \tag{A4}$$

in terms of the symplectic current (n-1)-form ω given by

$$\omega(\phi, \delta_1 \phi, \delta_2 \phi) \equiv \delta_1 \Theta(\phi, \delta_2 \phi) - \delta_2 \Theta(\phi, \delta_1 \phi). \tag{A5}$$

The symplectic current satisfies $d\omega(\phi, \delta_1\phi, \delta_2\phi) = \mathcal{E}'(\phi, \delta_2\phi)\delta_1\phi - \mathcal{E}'(\phi, \delta_1\phi)\delta_2\phi$ with $\mathcal{E}'(\phi, \delta\phi) \equiv \delta\mathcal{E}(\phi)$. Hence, $\omega(\phi, \delta_1\phi, \delta_2\phi)$ is closed for variations on solutions,

$$d\omega(\Phi, \delta_1 \Phi, \delta_2 \Phi) = 0 \tag{A6}$$

where Φ denotes ϕ restricted to satisfy $\mathcal{E}(\phi) = 0$, and $\delta\Phi$ denotes $\delta\phi$ restricted to satisfy $\mathcal{E}'(\Phi, \delta\phi) = 0$, i.e. $\delta\Phi$ is, formally, a tangent vector field on the space of solutions. Consequently, $\Omega_{\Sigma}(\phi, \delta_1\phi, \delta_2\phi)$ is unchanged by deformations of the spacelike surface Σ in any compact region of M.

In the previous constructions, a change of coordinates on M or E leaves $\mathcal{E}(\phi)$ unchanged [22], while $\Theta(\phi, \delta\phi)$ changes in general by an exact locally constructed (n-1)-form $d\nu(\phi, \delta\phi)$. However, one can show that [4] if the Lagrangian $L(\phi)$ is at most second order in partial derivatives $\partial^k \phi$ ($k \leq 2$) of ϕ , then $\Theta(\phi, \delta\phi)$ is independent of the choice of coordinates on M and E and thus the presymplectic form $\Omega_{\Sigma}(\phi, \delta_1 \phi, \delta_2 \phi)$ is then coordinate invariant.

Moreover, note that $L(\phi)$ can be freely changed by addition of a locally constructed exact form $d\mu(\phi)$, without affecting the field equations $\mathcal{E}(\phi)$. This changes $\Theta(\phi, \delta\phi)$ by addition of a locally constructed (n-1)-form $d\delta\mu(\phi)$, but leaves $\Omega_{\Sigma}(\phi, \delta_1\phi, \delta_2\phi)$ unchanged. Therefore, up to its dependence on Σ , the symplectic structure $\Omega_{\Sigma}(\phi, \delta_1\phi, \delta_2\phi)$ is uniquely determined by $\mathcal{E}(\phi)$ in this situation.

Now consider a complete, nowhere vanishing vector field ξ on M. It will be assumed that there exists a well-defined Lie derivative acting on ϕ associated to the diffeomorphism generated by ξ on M. Let Σ be a connected region contained in a fixed hypersurface in M with a closed boundary $\partial \Sigma$. (Note, if Σ is simply-connected, $\partial \Sigma$ is a closed n-2-surface in M bounding Σ . If Σ is multiply-connected, then $\partial \Sigma$ is a disjoint union of closed n-2-surfaces. Also, if Σ extends to "infinity", then $\partial \Sigma$ contains a corresponding "asymptotic boundary" n-2-surface.)

Definition A.1. A Hamiltonian conjugate to ξ on Σ is a function $H_{\Sigma}(\xi;\phi) = \int_{\Sigma} \mathcal{H}(\xi;\phi)$ for some locally constructed (n-1)-form $\mathcal{H}(\xi;\phi)$ such that, on solutions Φ ,

$$H'_{\Sigma}(\xi; \Phi, \delta\phi) = \Omega_{\Sigma}(\Phi, \delta\phi, \mathcal{L}_{\xi}\Phi) \tag{A7}$$

where \mathcal{L}_{ξ} denotes the Lie derivative, and $H'_{\Sigma}(\xi;\phi,\delta\phi) \equiv \delta H_{\Sigma}(\xi;\phi)$.

This is a covariant formulation of the standard Hamiltonian symplectic structure, with the "time" direction defined by ξ , called the *time flow* vector field. (In particular, Ref. [4] outlines a construction of a standard phase space and Hamiltonian equations of motion determined from this covariant structure.) Note that a Hamiltonian, if it exists, is automatically conserved along ξ for solutions Φ , i.e. $\mathcal{L}_{\xi}H_{\Sigma}(\xi;\Phi)=0$. It will now be shown that when ξ is a "time symmetry" of the Lagrangian $L(\phi)$, then a Hamiltonian conjugate to ξ exists and is simply given by the Noether charge associated to ξ .

Given any vector field ζ on M, consider the variation $\delta_{\zeta}\phi \equiv \mathcal{L}_{\zeta}\phi$. If this is a symmetry of the Lagrangian, so that

$$\delta_{\zeta}L(\phi) = L'(\phi, \mathcal{L}_{\zeta}\phi) = d(i_{\zeta}L(\phi)) = \mathcal{L}_{\zeta}L(\phi)$$
(A8)

by means of the identity $\mathcal{L}_{\zeta}L(\phi) = d(i_{\zeta}L(\phi))$, then one can define a conserved *Noether* current (n-1)-form $J(\zeta;\phi)$ by

$$J(\zeta;\phi) = \Theta(\phi, \mathcal{L}_{\zeta}\phi) - i_{\zeta}L(\phi) \tag{A9}$$

where i_{ζ} is the interior product. Conservation of this current simply means that, on solutions Φ , $J(\zeta;\phi)$ is closed

$$dJ(\zeta;\Phi) = d\Theta(\Phi, \mathcal{L}_{\zeta}\Phi) - d(i_{\zeta}L(\Phi)) = L'(\Phi, \delta\Phi) - \mathcal{L}_{\zeta}L(\Phi) = 0$$
(A10)

through the symmetry condition (A8). The integral of $J(\zeta; \Phi)$ over Σ defines the *Noether charge*

$$Q_{\Sigma}(\zeta) = \int_{\Sigma} J(\zeta; \Phi). \tag{A11}$$

One finds that the "time" derivative of this charge with respect to ξ is given by

$$\mathcal{L}_{\xi}Q_{\Sigma}(\zeta) = \int_{\Sigma} \mathcal{L}_{\xi}J(\zeta;\Phi) = \int_{\Sigma} i_{\xi}dJ(\zeta;\Phi) + d(i_{\xi}J(\zeta;\Phi)) = \oint_{\partial\Sigma} i_{\xi}J(\zeta;\Phi)$$
(A12)

where $i_{\xi}J(\zeta;\phi)$ is called the *flux* of the Noether current. Hence, if the flux vanishes on $\partial\Sigma$, then the charge is conserved for solutions Φ .

Examples of field theories which admit a symmetry $\delta_{\zeta}\phi = \mathcal{L}_{\zeta}\phi$ are (i) any generally-covariant theory on a fixed, background spacetime (M,g) with an isometry vector field ζ (i.e. $\mathcal{L}_{\zeta}g = 0$), where $L(\phi)$ is purely a function of g, ϕ and its metric-covariant derivatives $\nabla \phi$; (ii) any diffeomorphism-covariant theory, whose field variables ϕ include the spacetime metric g, where $L(\phi)$ is purely a function of ϕ , curvature tensor of g, and their metric-covariant derivatives.

For a diffeomorphism-covariant theory, $\delta_{\zeta}\phi$ is a symmetry for all vector fields ζ . Consequently, since $J(\zeta;\phi)$ is locally constructed out of ζ , one can show that in this case [4]

$$J(\zeta; \Phi) = dQ(\zeta; \Phi) \tag{A13}$$

for some locally constructed (n-2)-form $Q(\zeta;\phi)$, called the Noether current potential. Then the Noether charge reduces to a surface integral

$$Q_{\Sigma}(\zeta) = \int_{\Sigma} J(\zeta; \phi) = \oint_{\partial \Sigma} Q(\zeta; \phi). \tag{A14}$$

In contrast, for a generally-covariant theory, $J(\zeta; \Phi)$ is related to the conserved stress-energy tensor $T(\phi)$ defined by considering variations of g,

$$*\delta_g L(\phi) = -\frac{1}{2} T(\phi) \delta g + *d\Theta(\phi, \delta g). \tag{A15}$$

One can show that [9], on solutions Φ ,

$$J(\zeta; \Phi) = *i_{\zeta} T(\Phi) + d\tau(\zeta; \Phi)$$
(A16)

for some locally constructed (n-2)-form $\tau(\zeta;\phi)$.

Proposition A.2. For any symmetry $\delta_{\zeta}\phi = \mathcal{L}_{\zeta}\phi$ admitted by a Lagrangian $L(\phi)$, the field equations and symplectic potential satisfy

$$\delta_{\zeta} \mathcal{E}(\phi) = \mathcal{L}_{\zeta} \mathcal{E}(\phi), \tag{A17}$$

$$\delta_{\zeta}\Theta(\phi,\delta\phi) = \mathcal{L}_{\zeta}\Theta(\phi,\delta\phi) + d\psi(\zeta;\phi,\delta\phi) \tag{A18}$$

where $\psi(\zeta; \phi, \delta\phi)$ is some locally constructed (n-2)-form.

Proof:

Consider an arbitrary variation of the Lagrangian symmetry condition (A8),

$$0 = \delta(\delta_{\zeta}L(\phi) - \mathcal{L}_{\zeta}L(\phi)) = \delta_{\zeta}\delta L(\phi) - \mathcal{L}_{\zeta}\delta L(\phi). \tag{A19}$$

From Eq. (A3), one has

$$\mathcal{L}_{\zeta}(\delta L(\phi)) = \mathcal{L}_{\zeta}(\mathcal{E}(\phi)\delta\phi) + \mathcal{L}_{\zeta}d\Theta(\phi,\delta\phi) = (\mathcal{L}_{\zeta}\mathcal{E}(\phi))\delta\phi + \mathcal{E}(\phi)\delta\mathcal{L}_{\zeta}\phi + d\mathcal{L}_{\zeta}\Theta(\phi,\delta\phi), \quad (A20)$$

and similarly

$$\delta_{\zeta}(\delta L(\phi)) = (\delta_{\zeta} \mathcal{E}(\phi))\delta\phi + \mathcal{E}(\phi)\delta\mathcal{L}_{\zeta}\phi + d\delta_{\zeta}\Theta(\phi, \delta\phi), \tag{A21}$$

since $\delta_{\zeta}\phi = \mathcal{L}_{\zeta}\phi$. Hence, Eq. (A19) yields

$$(\delta_{\mathcal{C}}\mathcal{E}(\phi) - \mathcal{L}_{\mathcal{C}}\mathcal{E}(\phi))\delta\phi = d(\mathcal{L}_{\mathcal{C}}\Theta(\phi, \delta\phi) - \delta_{\mathcal{C}}\Theta(\phi, \delta\phi))$$
(A22)

holding for all $\delta\phi$. By taking $\delta\phi$ to have compact support and integrating the equation (A22) over M, one obtains $\int_M (\delta_\zeta \mathcal{E}(\phi) - \mathcal{L}_\zeta \mathcal{E}(\phi)) \delta\phi = 0$ which immediately yields Eq. (A17). Then Eq. (A22) shows that $\mathcal{L}_\zeta\Theta(\phi,\delta\phi) - \delta_\zeta\Theta(\phi,\delta\phi)$ is a closed (n-1)-form holding for all ϕ . Since this expression is locally constructed in terms of ϕ , it follows that [21,22] Eq. (A18) holds. \square

From these results, one finds that the variation of the Noether current is given by

$$J'(\zeta;\phi,\delta\phi) \equiv \delta J(\zeta;\phi) = \delta\Theta(\phi,\mathcal{L}_{\zeta}\phi) - i_{\zeta}\delta L(\phi)$$

$$= \omega(\phi,\delta\phi,\mathcal{L}_{\zeta}\phi) + \delta_{\zeta}\Theta(\phi,\delta\phi) - i_{\zeta}(d\Theta(\phi,\delta\phi) + \mathcal{E}(\phi)\delta\phi)$$

$$= \omega(\phi,\delta\phi,\mathcal{L}_{\zeta}\phi) - i_{\zeta}(\mathcal{E}(\phi)\delta\phi) + d(i_{\zeta}\Theta(\phi,\delta\phi) + \psi(\zeta;\phi,\delta\phi)) \quad (A23)$$

using the identity $i_{\zeta}(d\Theta(\phi,\delta\phi)) = \mathcal{L}_{\zeta}\Theta(\phi,\delta\phi) - d(i_{\zeta}\Theta(\phi,\delta\phi)).$

Lemma A.3. On solutions Φ ,

$$\Omega_{\Sigma}(\Phi, \mathcal{L}_{\zeta}\Phi, \delta\phi) = -\int_{\Sigma} J'(\zeta; \Phi, \delta\phi) + \oint_{\partial \Sigma} i_{\zeta}\Theta(\Phi, \delta\phi) + \psi(\zeta; \Phi, \delta\phi). \tag{A24}$$

Thus, for variations $\delta \phi$ with compact support in the interior of Σ , i.e. $\delta \phi|_{\partial \Sigma} = 0$,

$$\Omega_{\Sigma}(\Phi, \mathcal{L}_{\zeta}\Phi, \delta\phi) = -\int_{\Sigma} J'(\zeta; \Phi, \delta\phi). \tag{A25}$$

One can then apply this result to the time flow vector field $\zeta = \xi$ to obtain a Hamiltonian.

Theorem A.4. The Noether current $J(\xi;\phi)$ yields a Hamiltonian conjugate to ξ on Σ given by $H_{\Sigma}(\xi;\phi) = \int_{\Sigma} J(\xi;\phi)$ under compact support variations $\delta\phi$. For solutions Φ , $H_{\Sigma}(\xi;\Phi) = Q_{\Sigma}(\xi)$ is the conserved Noether charge associated to ξ .

For variations $\delta \phi$ without compact support, there exists a Hamiltonian if and only if one can find a locally constructed (n-2)-form $B(\xi;\phi)$ such that

$$\oint_{\partial \Sigma} B'(\xi; \Phi, \delta\phi) - i_{\xi} \Theta(\Phi, \delta\phi) - \psi(\xi; \Phi, \delta\phi) = 0$$
(A26)

where $B'(\xi; \phi, \delta \phi) \equiv \delta B(\xi; \phi)$. If one restricts to variations $\delta \phi = \delta \Phi$, then by considering a second variation and antisymmetrizing in this equation, one obtains the necessary condition

$$\oint_{\partial\Sigma} \delta_1(i_{\xi}\Theta(\Phi, \delta_2\Phi) + \psi(\xi; \Phi, \delta_2\Phi)) - \delta_2(i_{\xi}\Theta(\Phi, \delta_1\Phi) + \psi(\xi; \Phi, \delta_1\Phi)) = 0$$
(A27)

for existence of $B(\xi;\phi)$. This condition can also be shown to be sufficient [10].

Definition A.5. An allowed boundary condition on ϕ is a set of field components $\mathcal{F}(\phi)|_{\partial\Sigma}$ locally constructed from ϕ , partial derivatives $\partial^k \phi$, and spacetime quantities associated to $\xi, \Sigma, \partial\Sigma$, such that for all variations $\delta\phi$ satisfying $\mathcal{F}'(\phi, \delta\phi)|_{\partial\Sigma} = 0$, where $\mathcal{F}'(\phi, \delta\phi) \equiv \delta\mathcal{F}(\phi)$, there exists a Hamiltonian $H_{\Sigma}(\xi; \phi)$ conjugate to ξ on Σ .

One now has the following main result.

Theorem A.6. A Hamiltonian conjugate to ξ on Σ exists under variations $\delta \phi$ without compact support if and only if

$$\oint_{\partial \Sigma} i_{\xi} \omega(\Phi, \delta_1 \Phi, \delta_2 \Phi) = \oint_{\partial \Sigma} \psi'(\xi; \Phi, \delta_1 \Phi, \delta_2 \Phi)$$
(A28)

on solutions Φ , where $\psi'(\xi; \phi, \delta_1 \phi, \delta_2 \phi) \equiv \delta_1 \psi(\xi; \phi, \delta_2 \phi) - \delta_2 \psi(\xi; \phi, \delta_1 \phi)$. This determines the allowed boundary conditions $\mathcal{F}(\phi)|_{\partial \Sigma}$ for the field equations to admit a covariant Hamiltonian formulation. Then the Hamiltonian is

$$H_{\Sigma}(\xi;\phi) = \int_{\Sigma} J(\xi;\phi) - dB(\xi;\phi)$$
 (A29)

with $B(\xi;\phi)$ given by Eq. (A26) up to an arbitrary function of the boundary data $\mathcal{F}(\phi)$ and ξ . Furthermore, under the allowed boundary conditions, the Hamiltonian and symplectic structure are independent of choice of Σ .

The surface integral $\oint_{\partial\Sigma} i_{\xi}\omega(\Phi, \delta_1\Phi, \delta_2\Phi)$ will be referred to as the *symplectic flux* through $\partial\Sigma$.

For a diffeomorphism-covariant theory, or a generally-covariant theory on a background spacetime, one can show that $\psi(\xi;\phi,\delta\phi)\equiv 0$. Hence the necessary and sufficient condition for existence of a Hamiltonian becomes

$$\oint_{\partial \Sigma} i_{\xi} \omega(\Phi, \delta_1 \Phi, \delta_2 \Phi) = 0 \tag{A30}$$

and, furthermore, from the relation (A26) between $\Theta(\Phi, \delta\phi)$ and $B(\xi; \phi)$, it follows that one has

$$B(\xi;\phi)|_{\partial\Sigma} = (i_{\xi}\tilde{B}(\phi))|_{\partial\Sigma} \tag{A31}$$

where $\tilde{B}(\phi)$ is a locally constructed (n-1)-form. Then on solutions Φ the Hamiltonian takes the following form: in the case of a diffeomorphism-covariant theory,

$$H_B(\xi;\Phi) = \oint_{\partial\Sigma} Q(\xi;\Phi) - i_{\xi}\tilde{B}(\Phi)$$
 (A32)

which is a surface integral; and in the case of a generally-covariant theory,

$$H(\xi; \Phi) + H_B(\xi; \Phi) = \int_{\Sigma} *i_{\zeta} T(\Phi) + \oint_{\partial \Sigma} \tau(\xi; \Phi) - i_{\xi} \tilde{B}(\Phi)$$
 (A33)

where $H(\xi; \Phi) = \int_{\Sigma} *i_{\zeta} T(\Phi)$ is the canonical energy associated to Φ on Σ , and $H_B(\xi; \Phi)$ is the surface integral term.

To conclude, some further features of the Noether charge Hamiltonian will now be developed.

Definition A.7. The coefficient of an arbitrary compact support variation $\delta\phi|_{\Sigma}$ in the equation

$$\int_{\Sigma} \Omega_{\Sigma}(\phi, \delta\phi, \mathcal{L}_{\xi}\phi) - H'_{\Sigma}(\xi; \phi, \delta\phi) \equiv \int_{\Sigma} \mathcal{E}_{H}(\xi; \phi)\delta\phi = 0$$
(A34)

yields the Hamiltonian field equations for ϕ , $\mathcal{E}_H(\xi;\phi) = 0$.

Theorem A.8. The Hamiltonian field equations $\mathcal{E}_H(\xi;\phi) = 0$ are equivalent to the Lagrangian field equations $\mathcal{E}(\phi) = 0$.

Proof :

The Hamiltonian (A29) satisfies the variational identity

$$\Omega_{\Sigma}(\phi, \delta\phi, \mathcal{L}_{\xi}\phi) - H'_{\Sigma}(\xi; \phi, \delta\phi) = \int_{\Sigma} i_{\xi}(\mathcal{E}(\phi)\delta\phi)$$
(A35)

derived from Eqs. (A23) and (A26). Hence, for arbitrary compact support variations $\delta \phi|_{\Sigma}$, $\mathcal{E}(\phi) = 0$ holds if and only if ϕ satisfies $\mathcal{E}_H(\xi;\phi) = 0$. \square

A field variation, denoted by $\delta\phi_{\mathcal{N}}$, is a symplectic degeneracy direction if $\Omega_{\Sigma}(\phi, \delta\phi, \delta\phi_{\mathcal{N}}) = 0$ holds for arbitrary compact support variations $\delta\phi$. Such degeneracies arise whenever the Lagrangian $L(\phi)$ admits a gauge symmetry (i.e. a symmetry $\delta_{\chi}\phi$ that is locally constructed from ϕ , partial derivatives $\partial^k\phi$, and that depends linearly on a set of parameters χ freely specifiable as functions on M.) Note that the set $\{\delta\phi_{\mathcal{N}}\}$ of all degeneracy directions is a vector space. Then, a nondegeneracy direction, denoted by $\delta\phi_{\mathcal{D}}$, is represented as an equivalence class in the vector space of all field variations $\{\delta\phi\}$ quotiented by all symplectic degeneracy directions $\{\delta\phi_{\mathcal{N}}\}$, namely $\delta\phi_{\mathcal{D}} = \delta\phi/\delta\phi_{\mathcal{N}}$. This decomposition yields a break up of the Hamiltonian field equations (A34) into non-dynamical constraint equations,

$$H_{\Sigma}'(\xi;\phi,\delta\phi_{\mathcal{N}}) = 0, \tag{A36}$$

and dynamical evolution equations,

$$H'_{\Sigma}(\xi;\phi,\delta\phi_{\mathcal{D}}) = \Omega_{\Sigma}(\phi,\delta\phi_{\mathcal{D}},\mathcal{L}_{\xi}\phi), \tag{A37}$$

through arbitrary variations $\delta\phi_{\mathcal{N}}, \delta\phi_{\mathcal{D}}$ with compact support on Σ .

Since it assumed that the set $\{\phi\}$ of all fields has a linear (vector bundle) structure, the symplectic degeneracy directions $\delta\phi_{\mathcal{N}}$ can be identified with a corresponding set of field components, denoted $\phi_{\mathcal{N}}$, which will be called non-dynamical with respect to Σ . Similarly, the nondegeneracy directions $\delta\phi_{\mathcal{D}}$ determine a set of equivalence classes of field components, denoted $\phi_{\mathcal{D}}$, which will be called dynamical with respect to Σ . (Note these components $\phi_{\mathcal{D}}$ and $\phi_{\mathcal{N}}$ are locally constructed from ϕ , partial derivatives $\partial^k \phi$, and spacetime quantities associated to Σ .) Then, from the Hamiltonian variational identity (A35), one can view the constraint equations (A36) and evolution equations (A37) as arising equivalently through the action principle (A1) by variations with respect to $\phi_{\mathcal{N}}$ and $\phi_{\mathcal{D}}$.

In summary, the Noether charge formalism presented here gives a covariant Hamiltonian formulation for Lagrangian field theories in the situation where the underlying time flow is given by a symmetry of the Lagrangian.

REFERENCES

- [1] T. Regge and C. Teitelboim, "Role of surface integrals in the Hamiltonian Formulation of General Relativity", Annals of Physics 88 (1974) 286-318.
- [2] R. Arnowitt, S. Deser, C.W. Misner, "The Dynamics of General Relativity", in *Gravitation: An Introduction to Current Research* ed. L. Witten (New York: Wiley) (1962).
- [3] C. Crnković and E. Witten, in *Three Hundred Years of Gravitation*, ed. S.W. Hawking and W. Israel (Cambridge University Press: Cambridge) (1987) p.676-684.
- [4] J. Lee and R.M. Wald, "Local symmetries and constraints", J. Math. Phys. **31**, (1990) 725-743.
- [5] M. Gotay, J. Isenberg, and J. E. Marsden, "Momentum Maps and Classical Relativistic Fields", Part I (1997); Part II (1999), Unpublished Notes.
- [6] J. M. Nester, "A Covariant Hamiltonian for Gravity Theories", Mod. Phys. Lett. A 6, (1991) 2655-2661; J. M. Nester, "Some Progress in Canonical Gravity", in Directions in General Relativity, ed. B. L. Hu, M. P. Ryan and C. V. Vishveshwara (Cambridge University Press: Cambridge) Vol 1 (1993) 245-260.
- [7] J. Kijowski, "A Simple Derivation of Canonical Structure and Quasi-Local Hamiltonians in General Relativity", Gen. Relativ. Gravit. 29, (1997) 307-343; J. Kijowski and W.M. Tulczyjew, A Symplectic Framework for Field Theories, Lecture Notes in Physics No. 107 (Springer-Verlag: Berlin) (1979).
- [8] S.C. Anco and R.S. Tung, "Properties of the symplectic structure of General Relativity for spatially bounded spacetime regions", J. Math. Phys. 43, (2002) 3984-4019.
- [9] V. Iyer and R.M. Wald, "Some Properties of Noether Charge and a Proposal for Dynamical Black Hole Entropy", Phys. Rev. D **50**, (1994) 846-864.
- [10] R.M. Wald and A. Zoupas, "A General Definition of "Conserved Quantities" in General

- Relativity and Other Theories of Gravity", Phys. Rev. D 61, (2000) 084027.
- [11] V. Iyer and R.M. Wald, "A comparison of Noether charge and Euclidean methods for Computing the Entropy of Stationary Black Holes", Phys. Rev. D 52, (1995) 4430-4439.
- [12] R.M. Wald, General Relativity (University of Chicago Press: Chicago) (1984).
- [13] J.D. Jackson, Classical Electrodynamics (Wiley: New York) 2nd edition (1975).
- [14] R.M. Wald, "The first law of black hole mechanics", in *Directions in General Relativity* Volume 1, ed. B.L. Hu, M. Ryan, C.V. Vishveshwara, (Cambridge University Press: Cambridge), (1993).
- [15] J.W. York, "Boundary terms in the Action Principles of General Relativity", Found. Phys. 16, (1986) 249-257.
- [16] J.D. Brown and J.W. York, "Quasilocal energy and conserved charges derived from the gravitational action", Phys. Rev. D 47, (1993) 1407-1419.
- [17] J.D. Brown, S.R. Lau, J.W. York, "Action and Energy of the Gravitational Field", Annals Phys. 297 (2002) 175-218.
- [18] C.M. Chen, J.M. Nester, R.S. Tung, "Quasilocal energy-momentum for geometric gravity theories", Phys. Lett. A **203** (1995), 5-11.
- [19] C.M. Chen and J.M. Nester, "Quasilocal quantities for GR and other theories of gravity", Class. Quant. Grav. **16** (1999), 1279-1304.
- [20] H. Friedrich and G. Nagy, "The Initial Boundary Value Problem for Einstein's Vacuum Field Equation", Comm. Math. Phys. 201 (1999) 619-655.
- [21] R.M. Wald, J. Math. Phys. **31** (1990) 2378-2384.
- [22] I.M. Anderson, "Introduction to the variational bicomplex" in Mathematical Aspects of Classical Field Theory, ed. M. Gotay, J. Marsden, V. Moncrief, Cont. Math. 132 (1992)

51-73.